Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

pH-metric Result

logP (XH2 2+)	-2.38	
logP (XH +)	-4.96	±2.15 (n=47)
logP (neutral X)	1.92	±0.01 (n=47)

18B-28002 Points 1 to 35

M15_octanol concentration factor	0.761
Carbonate	0.1910 mM
Acidity error	0.00862 mM

18B-28002 Points 36 to 72

M15_octanol concentration factor	0.839
Carbonate	0.2848 mM
Acidity error	-0.02801 mM

18B-28002 Points 73 to 106

M15_octanol concentration factor	0.903
Carbonate	0.2174 mM
Acidity error	0.16739 mM

Warnings and errors

Errors	None
Warnings	One or more logP values out of range

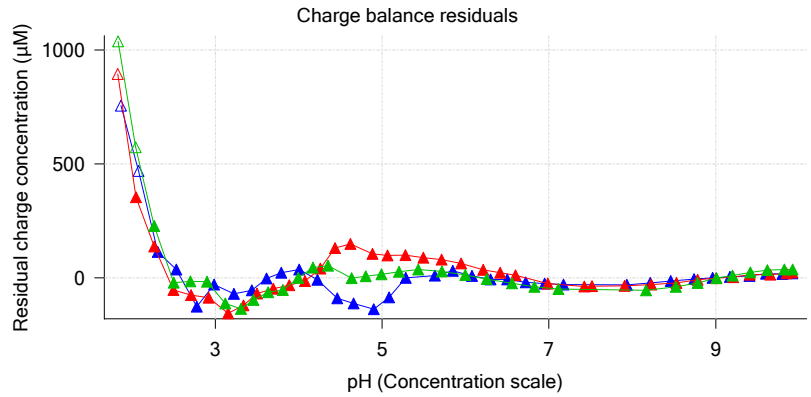
Sample logD and percent species

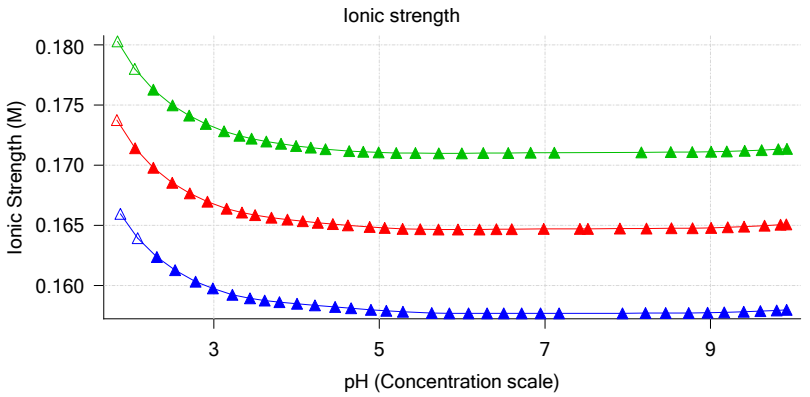
pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-2.38	97.03 %	2.55 %	0.00 %	0.40 %	0.00 %	0.01 %	
1.200	-2.37	95.59 %	3.98 %	0.00 %	0.40 %	0.00 %	0.03 %	Stomach pH
2.000	-1.92	78.23 %	20.58 %	0.01 %	0.33 %	0.00 %	0.86 %	
3.000	-0.52	21.05 %	55.37 %	0.28 %	0.09 %	0.00 %	23.22 %	
4.000	0.59	0.72 %	18.93 %	0.95 %	0.00 %	0.00 %	79.40 %	
5.000	1.45	0.01 %	2.30 %	1.15 %	0.00 %	0.00 %	96.54 %	
6.000	1.84	0.00 %	0.24 %	1.18 %	0.00 %	0.00 %	98.59 %	
6.500	1.90	0.00 %	0.07 %	1.18 %	0.00 %	0.00 %	98.75 %	
7.000	1.91	0.00 %	0.02 %	1.18 %	0.00 %	0.00 %	98.80 %	
7.400	1.92	0.00 %	0.01 %	1.18 %	0.00 %	0.00 %	98.81 %	Blood pH
8.000	1.92	0.00 %	0.00 %	1.18 %	0.00 %	0.00 %	98.82 %	
9.000	1.92	0.00 %	0.00 %	1.18 %	0.00 %	0.00 %	98.82 %	
10.000	1.92	0.00 %	0.00 %	1.18 %	0.00 %	0.00 %	98.82 %	
11.000	1.92	0.00 %	0.00 %	1.18 %	0.00 %	0.00 %	98.82 %	
12.000	1.92	0.00 %	0.00 %	1.18 %	0.00 %	0.00 %	98.82 %	

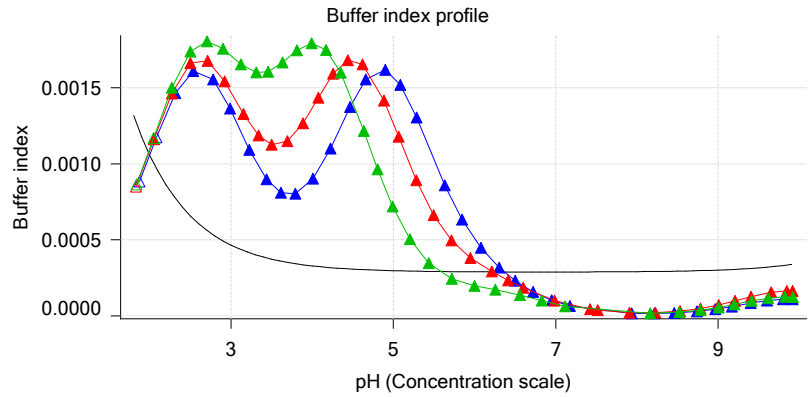
Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

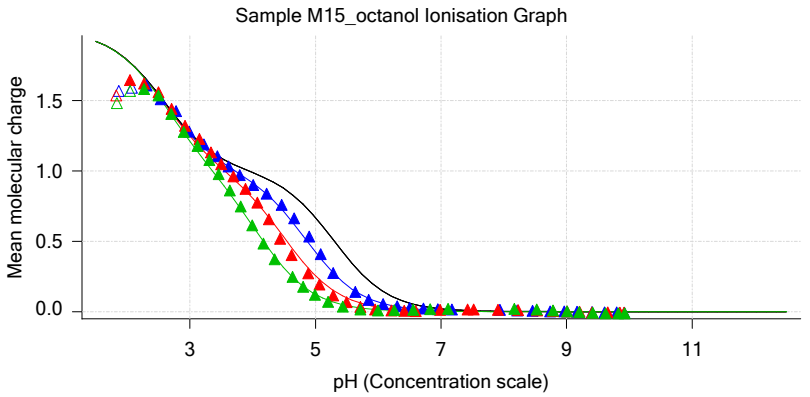
Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

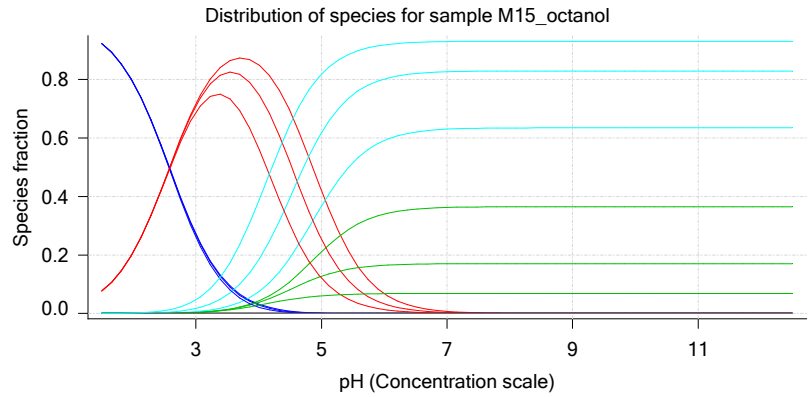
Graphs

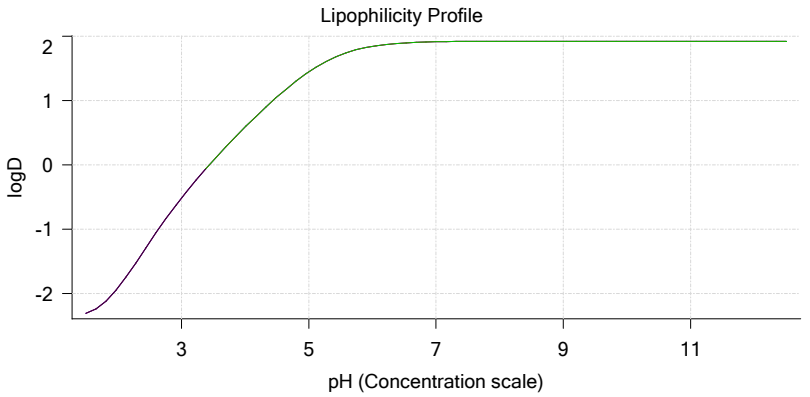


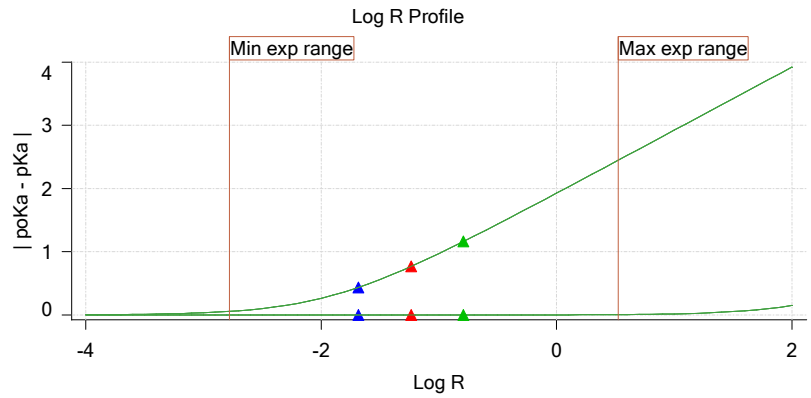


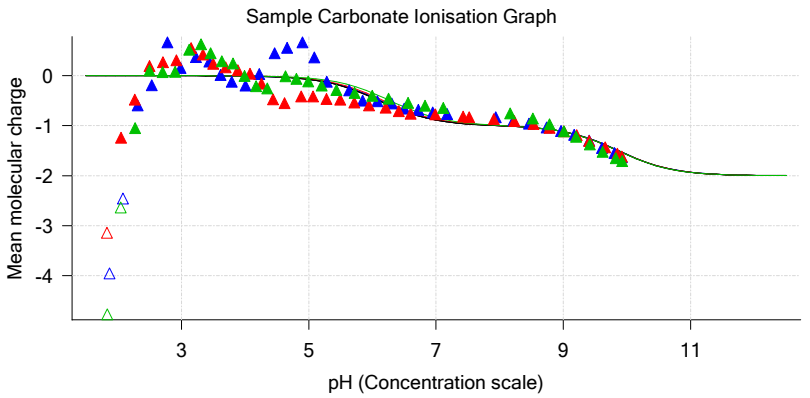








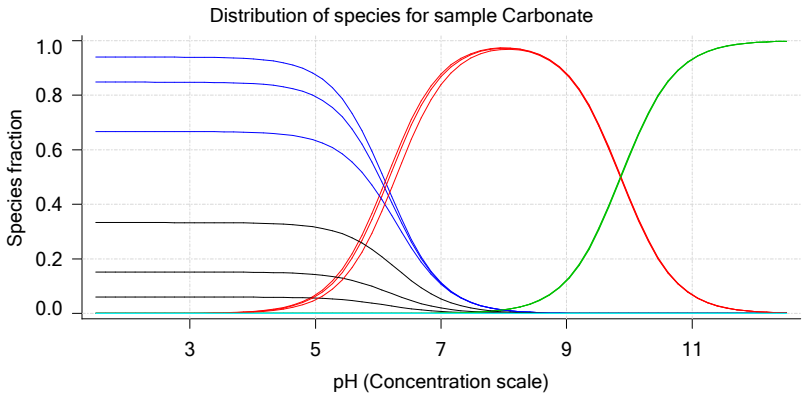




Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Graphs (continued)



Sample name:	**M15_octanol**	Experiment start time:	**2/28/2018 1:10:47 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-28002**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 1 of 3 18B-28002 Points 1 to 35

Overall results

RMSD	0.336
Average ionic strength	0.158 M
Average temperature	25.0°C
Partition ratio	0.0208 : 1
Analyte concentration range	3493.3 µM to 3618.9 µM
Total points considered	33 of 35

Warnings and errors

Errors	None
Warnings	One or more logP values out of range

Four-Plus parameters

Alpha	0.130	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r

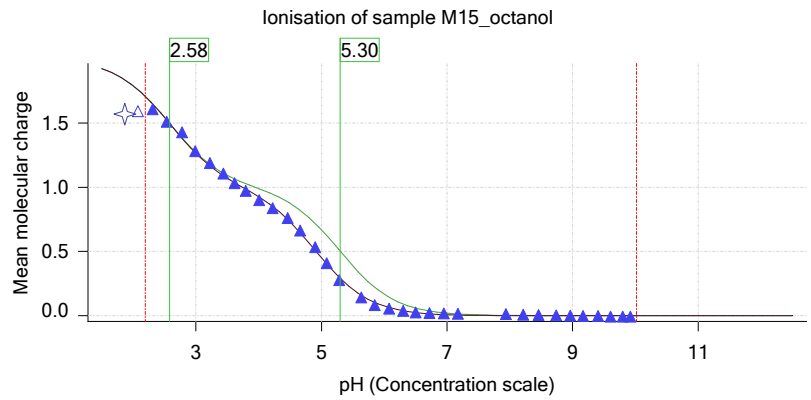
Titrants

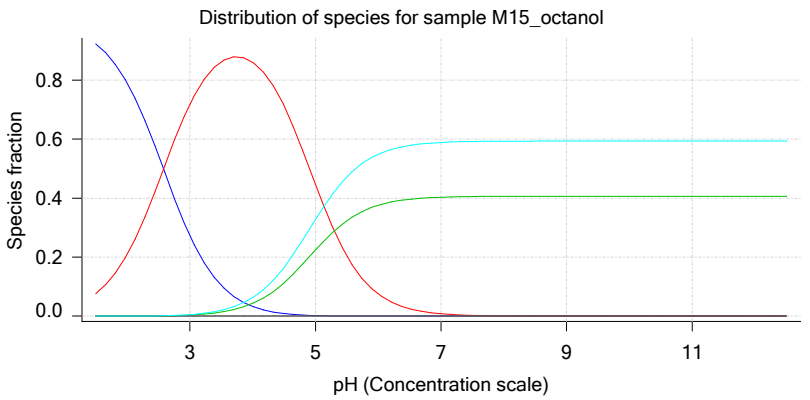
0.50 M HCl	0.993513	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/28/2018 1:10:47 AM	C:\Sirius_T3\KOH18B27.t3r

Sample

M15_octanol concentration factor	0.761
Base pKa 1	2.58
Base pKa 2	5.30
logP (XH2 2+)	-2.38
logP (XH +)	-9.58
logP (neutral X)	1.85

Sample graphs

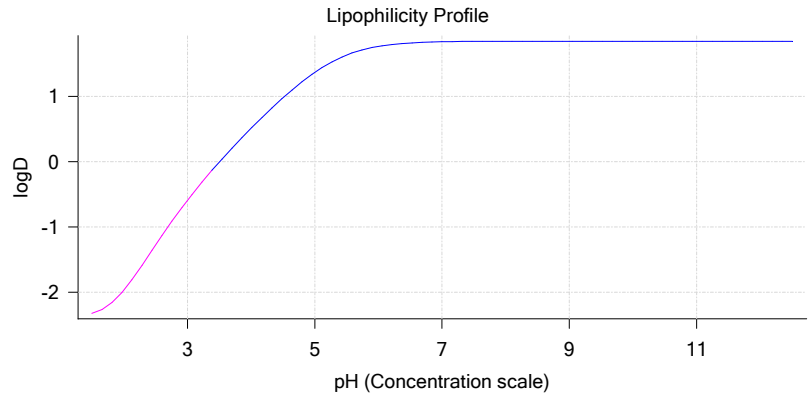




Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



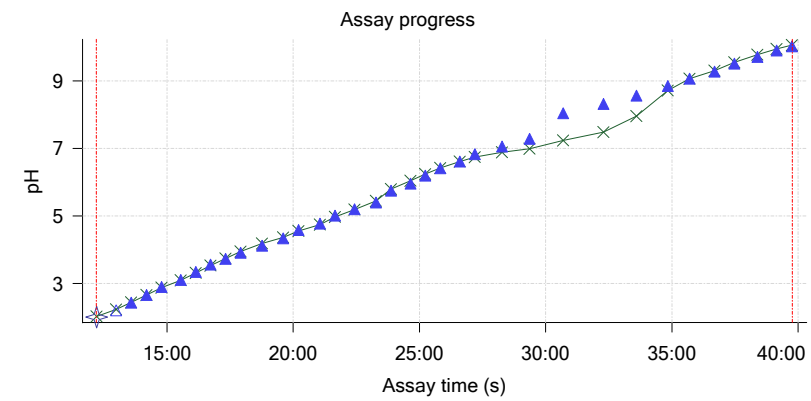
Sample logD and percent species

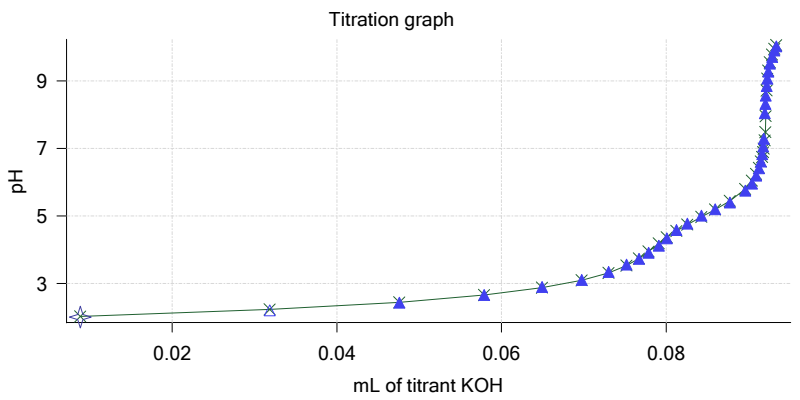
pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-2.38	97.43 %	2.56 %	0.00 %	0.01 %	0.00 %	0.00 %	
1.200	-2.37	95.99 %	4.00 %	0.00 %	0.01 %	0.00 %	0.00 %	Stomach pH
2.000	-1.97	79.15 %	20.82 %	0.01 %	0.01 %	0.00 %	0.02 %	
3.000	-0.59	27.30 %	71.81 %	0.36 %	0.00 %	0.00 %	0.53 %	
4.000	0.51	3.27 %	86.11 %	4.32 %	0.00 %	0.00 %	6.30 %	
5.000	1.37	0.17 %	44.71 %	22.41 %	0.00 %	0.00 %	32.72 %	
6.000	1.77	0.00 %	7.50 %	37.60 %	0.00 %	0.00 %	54.90 %	
6.500	1.82	0.00 %	2.50 %	39.63 %	0.00 %	0.00 %	57.87 %	
7.000	1.84	0.00 %	0.80 %	40.32 %	0.00 %	0.00 %	58.87 %	
7.400	1.84	0.00 %	0.32 %	40.52 %	0.00 %	0.00 %	59.16 %	Blood pH
8.000	1.85	0.00 %	0.08 %	40.62 %	0.00 %	0.00 %	59.30 %	
9.000	1.85	0.00 %	0.01 %	40.64 %	0.00 %	0.00 %	59.35 %	
10.000	1.85	0.00 %	0.00 %	40.65 %	0.00 %	0.00 %	59.35 %	
11.000	1.85	0.00 %	0.00 %	40.65 %	0.00 %	0.00 %	59.35 %	
12.000	1.85	0.00 %	0.00 %	40.65 %	0.00 %	0.00 %	59.35 %	

Carbonate and acidity

Carbonate 0.191 mM
Acidity error 0.009 mM

Other graphs

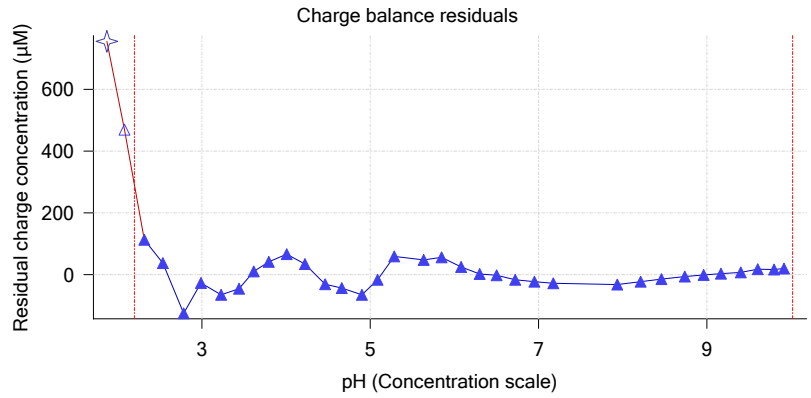


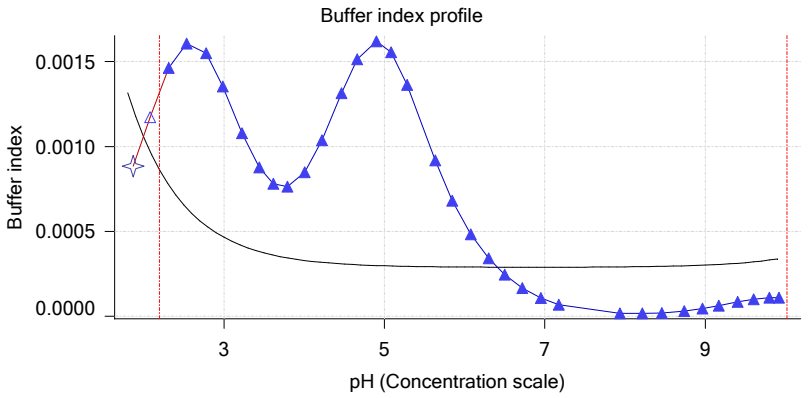


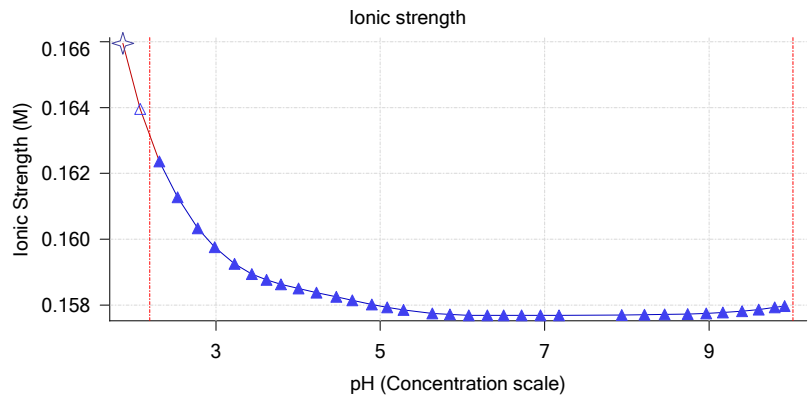
Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

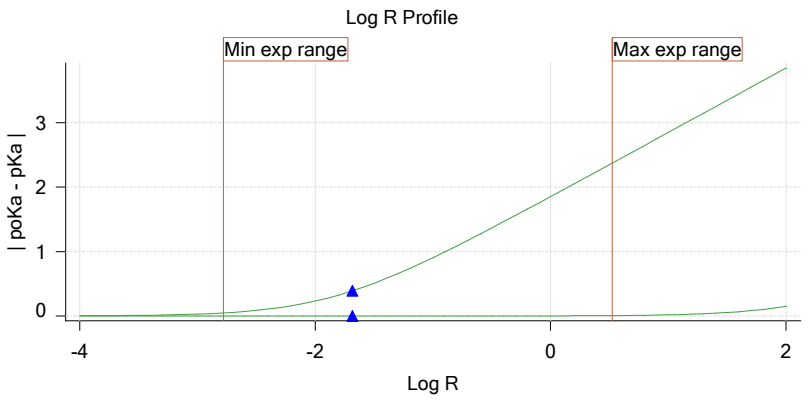
Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

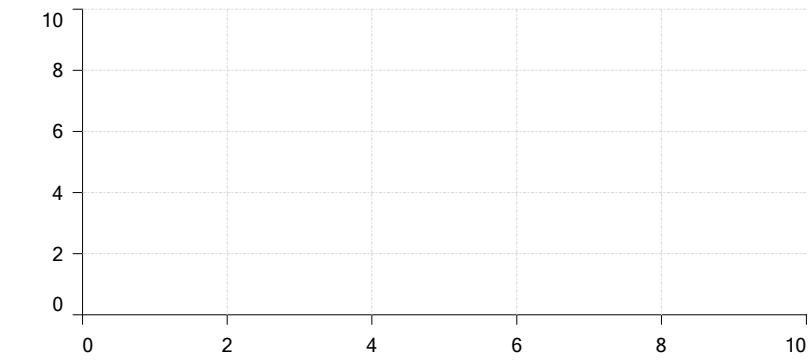
Other graphs (continued)

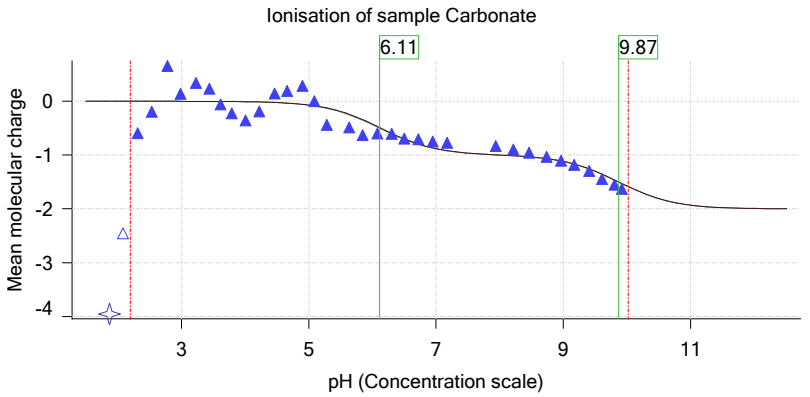












Sample name:	**M15_octanol**	Experiment start time:	**2/28/2018 1:10:47 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-28002**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 2 of 3 18B-28002 Points 36 to 72

Overall results

RMSD	0.387
Average ionic strength	0.166 M
Average temperature	25.0°C
Partition ratio	0.0581 : 1
Analyte concentration range	3113.6 µM to 3230.1 µM
Total points considered	36 of 37

Warnings and errors

Errors	None
Warnings	One or more logP values out of range

Four-Plus parameters

Alpha	0.130	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r

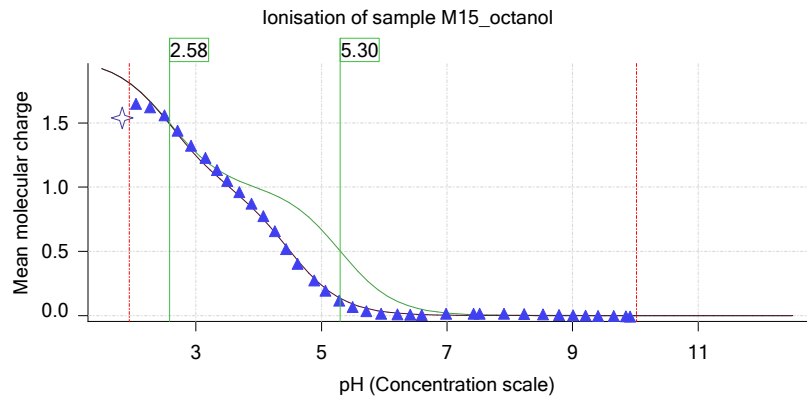
Titrants

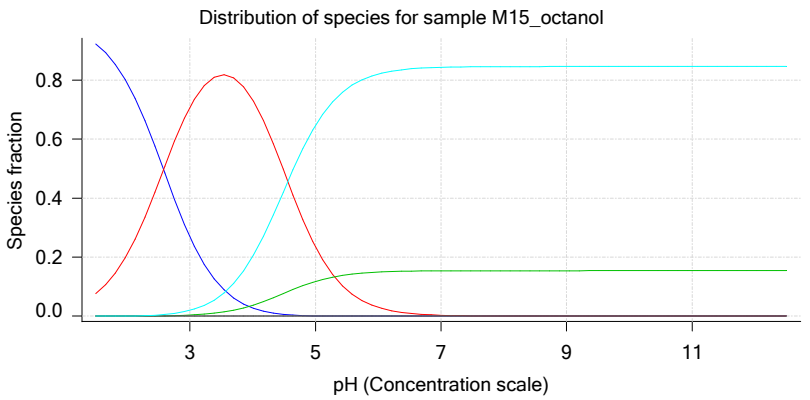
0.50 M HCl	0.993513	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/28/2018 1:10:47 AM	C:\Sirius_T3\KOH18B27.t3r

Sample

M15_octanol concentration factor	0.839
Base pKa 1	2.58
Base pKa 2	5.30
logP (XH2 2+)	-2.38
logP (XH +)	-3.43
logP (neutral X)	1.98

Sample graphs

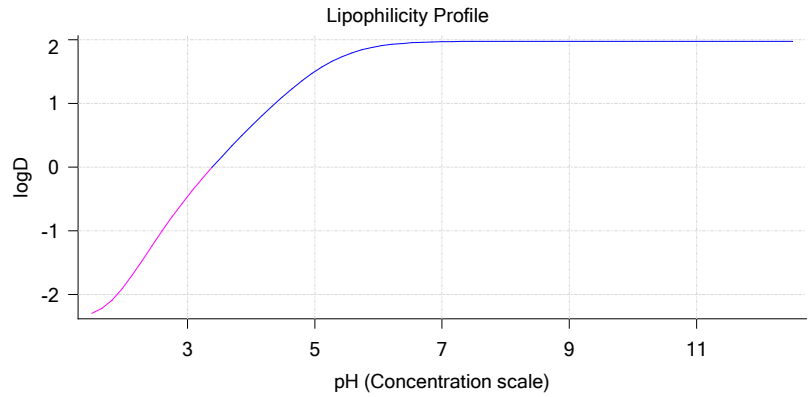




Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



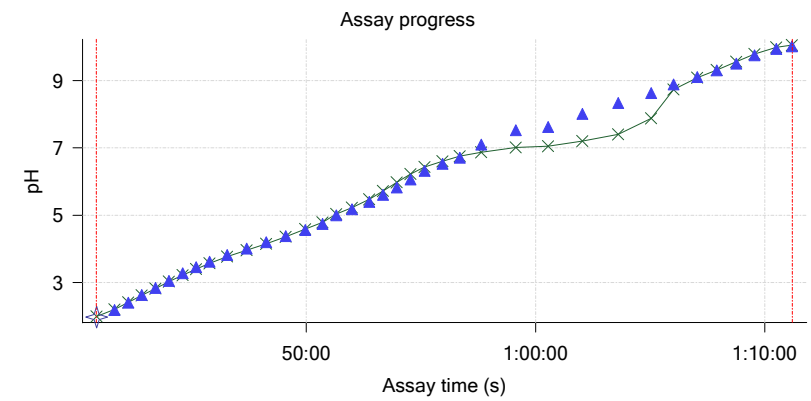
Sample logD and percent species

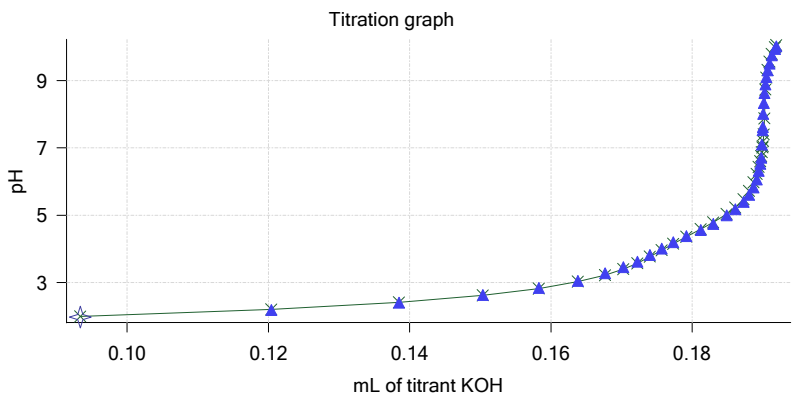
pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-2.38	97.41 %	2.56 %	0.00 %	0.02 %	0.00 %	0.00 %	
1.200	-2.36	95.97 %	4.00 %	0.00 %	0.02 %	0.00 %	0.00 %	Stomach pH
2.000	-1.88	79.11 %	20.81 %	0.01 %	0.02 %	0.00 %	0.06 %	
3.000	-0.46	26.91 %	70.78 %	0.35 %	0.01 %	0.00 %	1.95 %	
4.000	0.64	2.79 %	73.34 %	3.68 %	0.00 %	0.00 %	20.19 %	
5.000	1.50	0.09 %	23.48 %	11.77 %	0.00 %	0.00 %	64.66 %	
6.000	1.90	0.00 %	2.98 %	14.94 %	0.00 %	0.00 %	82.08 %	
6.500	1.95	0.00 %	0.96 %	15.25 %	0.00 %	0.00 %	83.79 %	
7.000	1.97	0.00 %	0.31 %	15.35 %	0.00 %	0.00 %	84.34 %	
7.400	1.97	0.00 %	0.12 %	15.38 %	0.00 %	0.00 %	84.50 %	Blood pH
8.000	1.97	0.00 %	0.03 %	15.39 %	0.00 %	0.00 %	84.57 %	
9.000	1.98	0.00 %	0.00 %	15.40 %	0.00 %	0.00 %	84.60 %	
10.000	1.98	0.00 %	0.00 %	15.40 %	0.00 %	0.00 %	84.60 %	
11.000	1.98	0.00 %	0.00 %	15.40 %	0.00 %	0.00 %	84.60 %	
12.000	1.98	0.00 %	0.00 %	15.40 %	0.00 %	0.00 %	84.60 %	

Carbonate and acidity

Carbonate 0.285 mM
Acidity error -0.028 mM

Other graphs

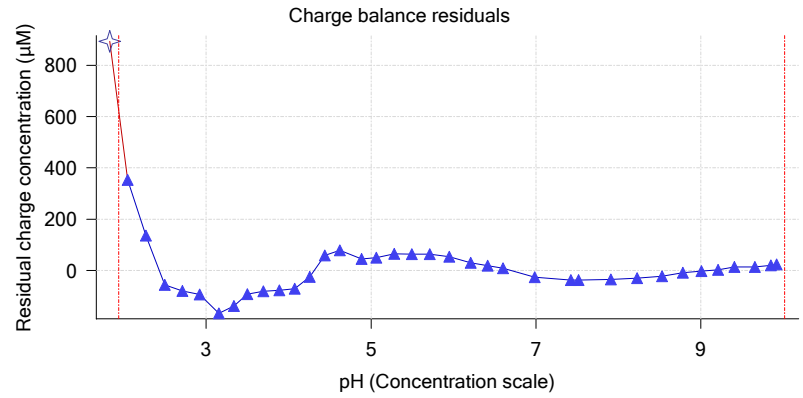


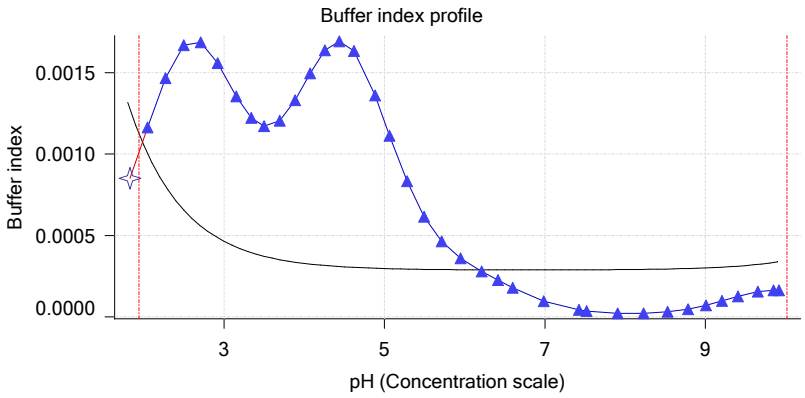


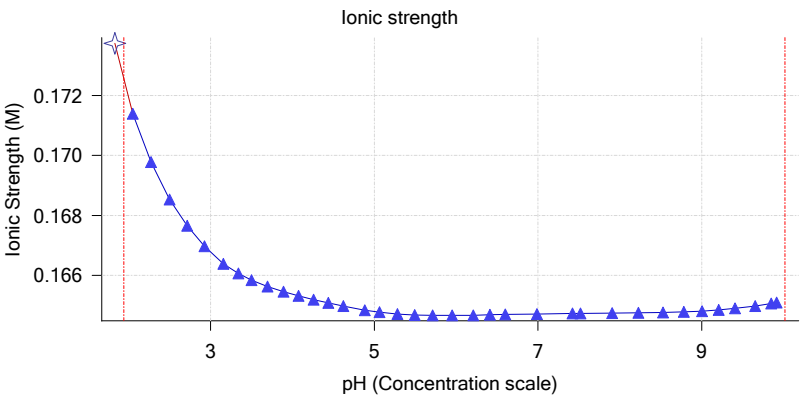
Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

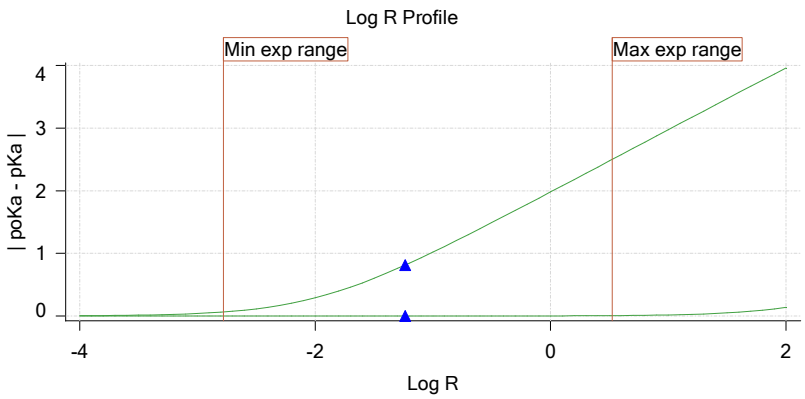
Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

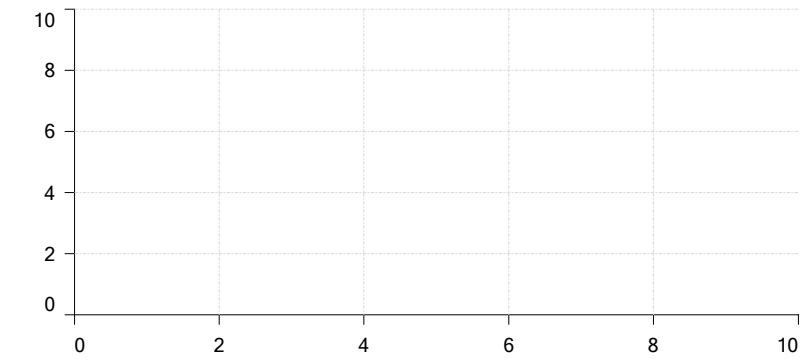
Other graphs (continued)

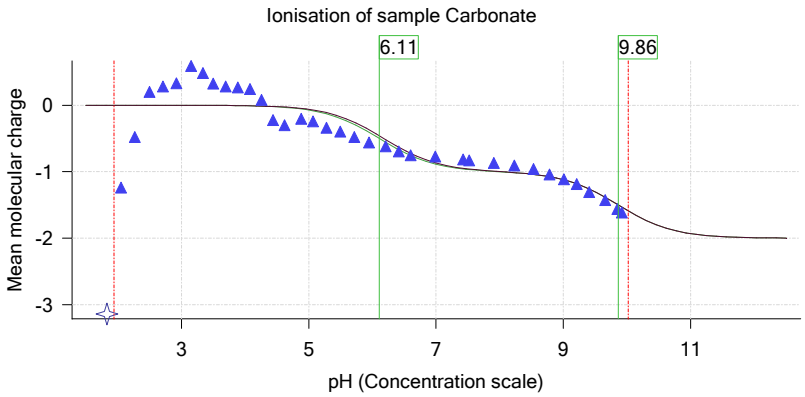












Sample name:	**M15_octanol**	Experiment start time:	**2/28/2018 1:10:47 AM**
Assay name:	**pH-metric high logP**	Analyst:	**Pion**
Assay ID:	**18B-28002**	Instrument ID:	**T312060**
Filename:	**C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**		

pH-metric high logP Titration 3 of 3 18B-28002 Points 73 to 106

Overall results

RMSD	0.501
Average ionic strength	0.172 M
Average temperature	25.0°C
Partition ratio	0.1616 : 1
Analyte concentration range	2625.5 µM to 2712.6 µM
Total points considered	32 of 34

Warnings and errors

Errors	None
Warnings	One or more logP values out of range

Four-Plus parameters

Alpha	0.130	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
S	0.9970	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
jH	0.8	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
jOH	-0.4	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r

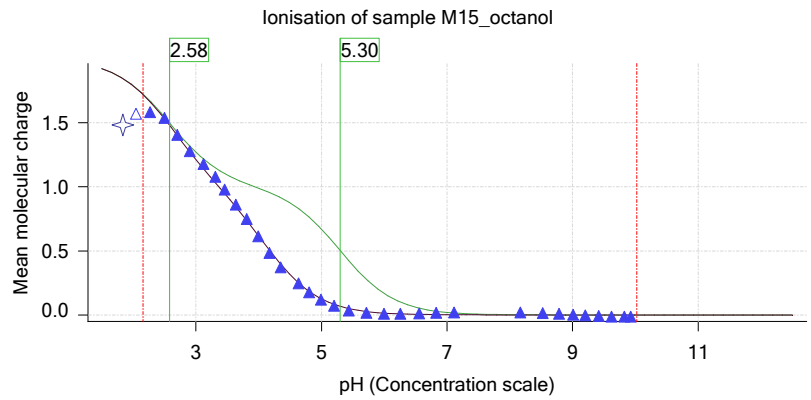
Titrants

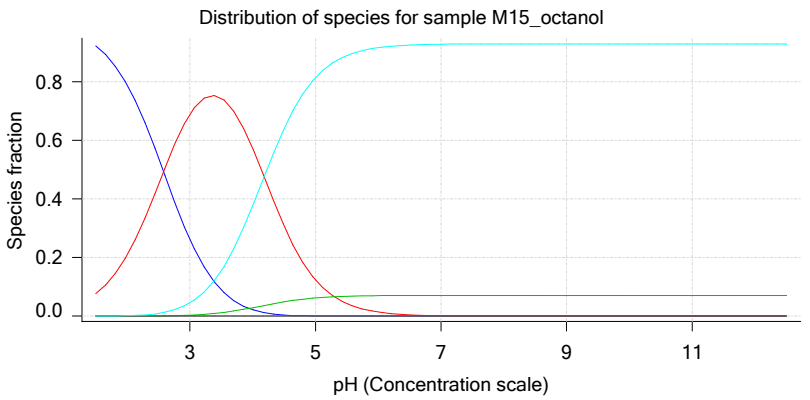
0.50 M HCl	0.993513	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
0.50 M KOH	0.999845	2/28/2018 1:10:47 AM	C:\Sirius_T3\KOH18B27.t3r

Sample

M15_octanol concentration factor	0.903
Base pKa 1	2.58
Base pKa 2	5.30
logP (XH2 2+)	-2.38
logP (XH +)	-3.95
logP (neutral X)	1.91

Sample graphs

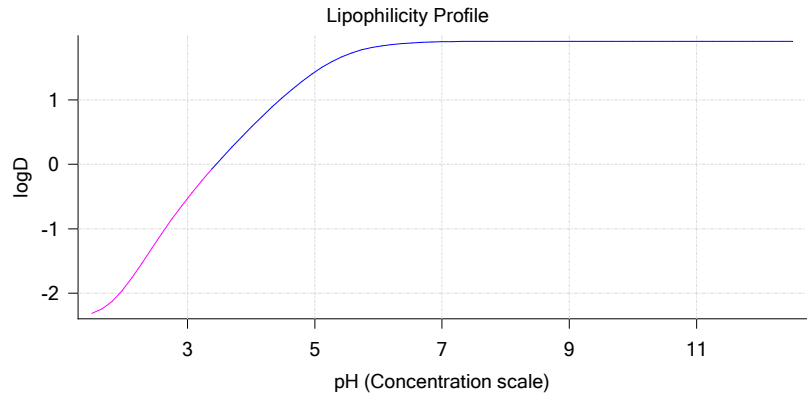




Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Sample graphs (continued)



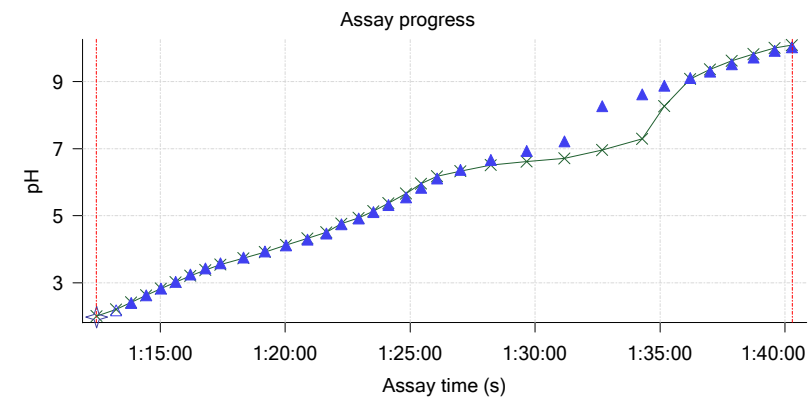
Sample logD and percent species

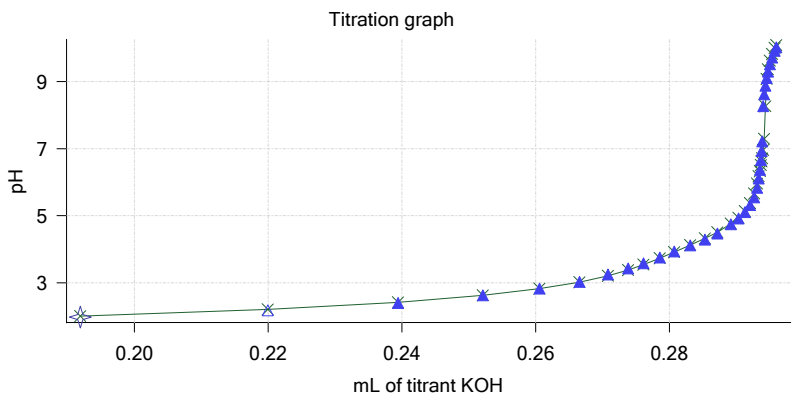
pH	M15_octanol logD	M15_octanol M15_octanolH2	M15_octanol M15_octanolH	M15_octanol M15_octanol	M15_octanol M15_octanolH2*	M15_octanol M15_octanolH*	M15_octanol M15_octanol*	Comment
1.000	-2.38	97.37 %	2.56 %	0.00 %	0.07 %	0.00 %	0.00 %	
1.200	-2.37	95.93 %	4.00 %	0.00 %	0.06 %	0.00 %	0.00 %	Stomach pH
2.000	-1.93	79.02 %	20.78 %	0.01 %	0.05 %	0.00 %	0.14 %	
3.000	-0.53	26.20 %	68.91 %	0.35 %	0.02 %	0.00 %	4.53 %	
4.000	0.57	2.18 %	57.29 %	2.87 %	0.00 %	0.00 %	37.65 %	
5.000	1.43	0.05 %	12.38 %	6.21 %	0.00 %	0.00 %	81.37 %	
6.000	1.83	0.00 %	1.39 %	6.99 %	0.00 %	0.00 %	91.62 %	
6.500	1.88	0.00 %	0.45 %	7.05 %	0.00 %	0.00 %	92.50 %	
7.000	1.90	0.00 %	0.14 %	7.08 %	0.00 %	0.00 %	92.78 %	
7.400	1.91	0.00 %	0.06 %	7.08 %	0.00 %	0.00 %	92.86 %	Blood pH
8.000	1.91	0.00 %	0.01 %	7.08 %	0.00 %	0.00 %	92.90 %	
9.000	1.91	0.00 %	0.00 %	7.09 %	0.00 %	0.00 %	92.91 %	
10.000	1.91	0.00 %	0.00 %	7.09 %	0.00 %	0.00 %	92.91 %	
11.000	1.91	0.00 %	0.00 %	7.09 %	0.00 %	0.00 %	92.91 %	
12.000	1.91	0.00 %	0.00 %	7.09 %	0.00 %	0.00 %	92.91 %	

Carbonate and acidity

Carbonate 0.217 mM
Acidity error 0.167 mM

Other graphs

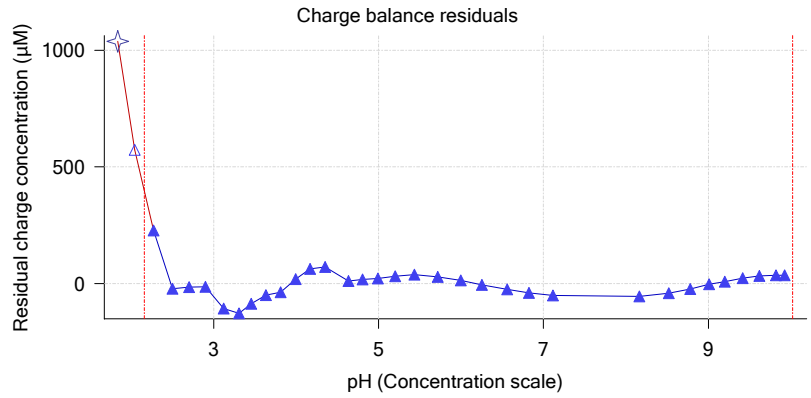


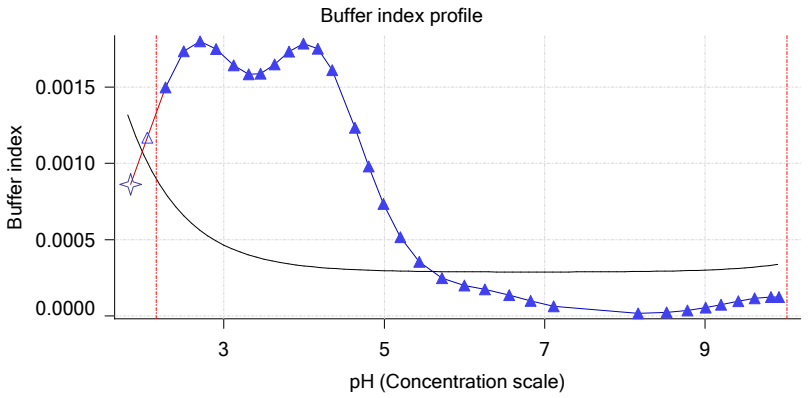


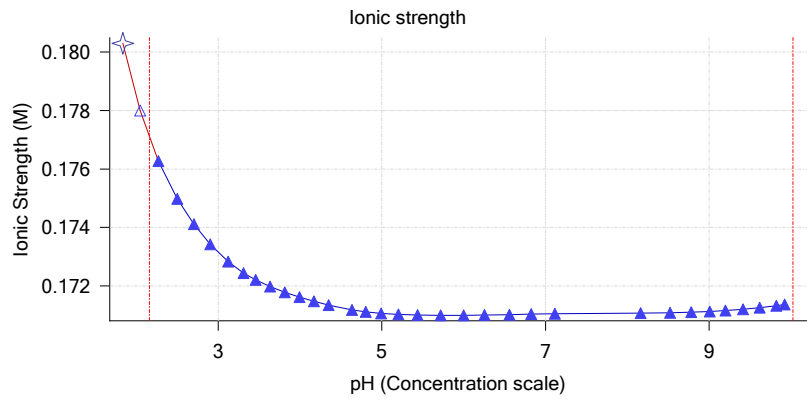
Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

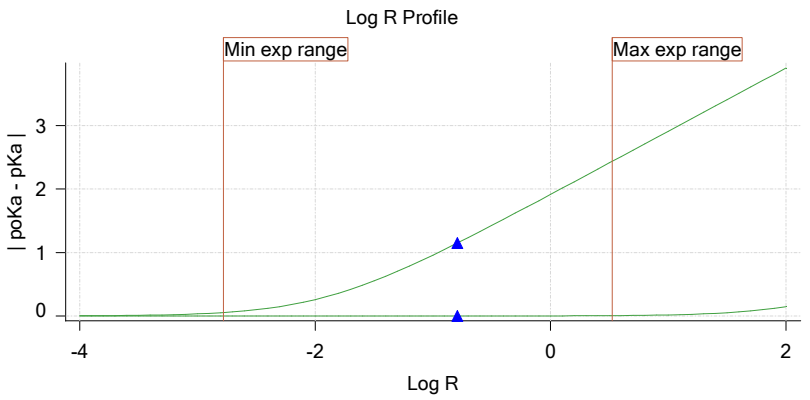
Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

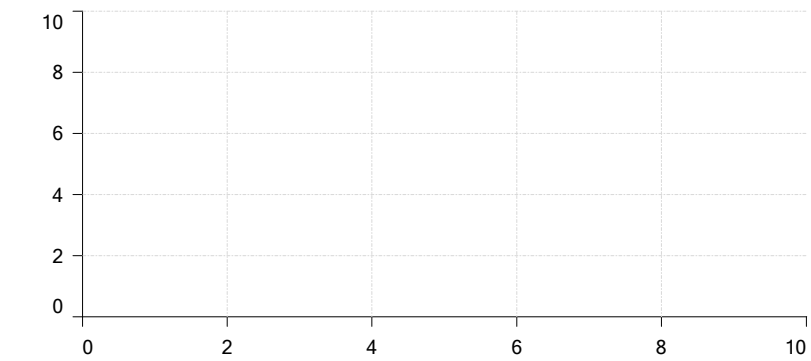
Other graphs (continued)

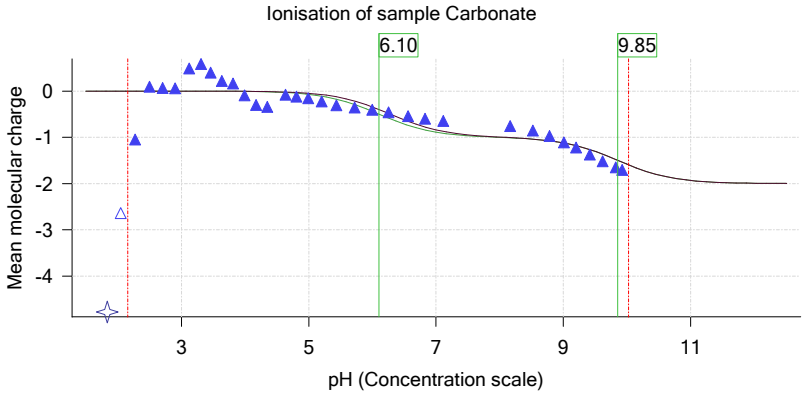












Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Model

Settings	Value	Date/Time changed	Imported from
Sample name	M15_octanol	2/27/2018 5:03:03 PM	User entered value
Sample by	Weight		Default value
Sample weight	0.001780 g	2/27/2018 6:41:09 PM	User entered value
Formula weight	209.25 g/mol	2/27/2018 5:03:03 PM	User entered value
Solubility	Unknown		Default value
Molecular weight	209.25	2/27/2018 5:03:03 PM	User entered value
Individual pKa ionic environments	No		Default value
Number of pKas	2	2/27/2018 5:03:03 PM	User entered value
Sample is a	Base	2/27/2018 5:03:03 PM	User entered value
pKa 1	2.58	2/27/2018 5:03:03 PM	User entered value
pKa 2	5.30	2/27/2018 5:03:03 PM	User entered value
logP (XH2 2+)	-2.38	2/27/2018 5:03:37 PM	User entered value
logp (XH +)	-1.38	2/27/2018 5:03:29 PM	User entered value
logP (neutral X)	1.33	2/27/2018 5:03:21 PM	User entered value

Events

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
9:12.2	Initial pH = 6.77									
12:12.8	Data point 1	2.20002 mL	0.09175 mL	0.00884 mL	0.05000 mL	2.005	-0.01157	0.40408	0.00090	10.0 s
12:59.2	Data point 2	2.20002 mL	0.09175 mL	0.03187 mL	0.05000 mL	2.209	-0.00700	0.51322	0.00048	10.0 s
13:35.0	Data point 3	2.20002 mL	0.09175 mL	0.04760 mL	0.05000 mL	2.439	-0.01430	0.68245	0.00086	10.5 s
14:11.1	Data point 4	2.20002 mL	0.09175 mL	0.05788 mL	0.05000 mL	2.658	-0.01104	0.75037	0.00063	10.0 s
14:46.7	Data point 5	2.20002 mL	0.09175 mL	0.06491 mL	0.05000 mL	2.903	-0.00268	0.03532	0.00070	10.0 s
15:32.6	Data point 6	2.20002 mL	0.09175 mL	0.06976 mL	0.05000 mL	3.109	0.00003	0.00001	0.00060	10.0 s
16:08.1	Data point 7	2.20002 mL	0.09175 mL	0.07300 mL	0.05000 mL	3.347	-0.00484	0.65284	0.00030	10.0 s
16:43.6	Data point 8	2.20002 mL	0.09175 mL	0.07516 mL	0.05000 mL	3.559	-0.01288	0.80904	0.00071	10.0 s
17:19.1	Data point 9	2.20002 mL	0.09175 mL	0.07669 mL	0.05000 mL	3.735	-0.00362	0.61081	0.00023	10.0 s
17:54.5	Data point 10	2.20002 mL	0.09175 mL	0.07787 mL	0.05000 mL	3.912	-0.00298	0.56183	0.00020	10.0 s
18:45.5	Data point 11	2.20002 mL	0.09175 mL	0.07909 mL	0.05000 mL	4.125	0.00402	0.19132	0.00045	10.0 s
19:36.3	Data point 12	2.20002 mL	0.09175 mL	0.08008 mL	0.05000 mL	4.341	-0.00621	0.78463	0.00035	10.5 s
20:12.2	Data point 13	2.20002 mL	0.09175 mL	0.08123 mL	0.05000 mL	4.581	-0.01069	0.76499	0.00060	10.0 s
21:03.2	Data point 14	2.20002 mL	0.09175 mL	0.08255 mL	0.05000 mL	4.776	-0.00334	0.62508	0.00021	10.5 s
21:39.2	Data point 15	2.20002 mL	0.09175 mL	0.08429 mL	0.05000 mL	5.014	0.00455	0.39258	0.00036	10.5 s
22:25.5	Data point 16	2.20002 mL	0.09175 mL	0.08596 mL	0.05000 mL	5.200	-0.00496	0.25675	0.00048	10.0 s
23:16.5	Data point 17	2.20002 mL	0.09175 mL	0.08772 mL	0.05000 mL	5.399	-0.01087	0.54074	0.00073	10.5 s
23:52.5	Data point 18	2.20002 mL	0.09175 mL	0.08958 mL	0.05000 mL	5.748	-0.00304	0.04364	0.00072	10.5 s
24:38.7	Data point 19	2.20002 mL	0.09175 mL	0.09043 mL	0.05000 mL	5.958	-0.00868	0.75112	0.00049	10.0 s
25:14.1	Data point 20	2.20002 mL	0.09175 mL	0.09092 mL	0.05000 mL	6.190	-0.01451	0.83075	0.00079	10.0 s
25:49.5	Data point 21	2.20002 mL	0.09175 mL	0.09125 mL	0.05000 mL	6.413	-0.01920	0.95433	0.00097	10.5 s
26:35.7	Data point 22	2.20002 mL	0.09175 mL	0.09151 mL	0.05000 mL	6.612	-0.01748	0.96637	0.00088	10.5 s
27:11.6	Data point 23	2.20002 mL	0.09175 mL	0.09165 mL	0.05000 mL	6.831	-0.01570	0.64440	0.00097	34.0 s
28:16.3	Data point 24	2.20002 mL	0.09175 mL	0.09177 mL	0.05000 mL	7.058	-0.01716	0.88880	0.00090	35.0 s
29:21.8	Data point 25	2.20002 mL	0.09175 mL	0.09184 mL	0.05000 mL	7.282	-0.01947	0.92580	0.00100	49.5 s
30:41.9	Data point 26	2.20002 mL	0.09175 mL	0.09196 mL	0.05000 mL	8.043	-0.03436	0.98140	0.00171	Timed out at 59.5 s
32:17.6	Data point 27	2.20002 mL	0.09175 mL	0.09203 mL	0.05000 mL	8.319	-0.01934	0.98179	0.00096	42.5 s
33:35.8	Data point 28	2.20002 mL	0.09175 mL	0.09210 mL	0.05000 mL	8.564	-0.01948	0.95892	0.00098	39.0 s
34:50.5	Data point 29	2.20002 mL	0.09175 mL	0.09219 mL	0.05000 mL	8.842	-0.01977	0.97108	0.00099	21.0 s
35:42.1	Data point 30	2.20002 mL	0.09175 mL	0.09229 mL	0.05000 mL	9.067	-0.01861	0.91683	0.00096	29.0 s
36:41.7	Data point 31	2.20002 mL	0.09175 mL	0.09240 mL	0.05000 mL	9.270	-0.01864	0.96902	0.00094	16.0 s
37:28.2	Data point 32	2.20002 mL	0.09175 mL	0.09259 mL	0.05000 mL	9.504	-0.01908	0.97520	0.00095	14.0 s
38:23.1	Data point 33	2.20002 mL	0.09175 mL	0.09285 mL	0.05000 mL	9.705	-0.01982	0.95760	0.00100	10.5 s
39:09.4	Data point 34	2.20002 mL	0.09175 mL	0.09313 mL	0.05000 mL	9.900	-0.01284	0.77555	0.00072	10.5 s
39:45.3	Data point 35	2.20002 mL	0.09175 mL	0.09337 mL	0.05000 mL	10.019	-0.01383	0.93336	0.00071	10.0 s
40:51.5	Data point 36	2.20002 mL	0.19015 mL	0.09337 mL	0.15000 mL	1.966	-0.01118	0.80408	0.00062	10.0 s
41:38.0	Data point 37	2.20002 mL	0.19015 mL	0.12041 mL	0.15000 mL	2.180	0.01132	0.58782	0.00073	10.0 s

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
42:13.9	Data point 38	2.20002 mL	0.19015 mL	0.13848 mL	0.15000 mL	2.397	-0.00623	0.18166	0.00072	10.0 s
42:49.6	Data point 39	2.20002 mL	0.19015 mL	0.15038 mL	0.15000 mL	2.623	-0.00443	0.19218	0.00050	10.0 s
43:25.2	Data point 40	2.20002 mL	0.19015 mL	0.15830 mL	0.15000 mL	2.834	-0.00869	0.46386	0.00063	10.0 s
44:00.8	Data point 41	2.20002 mL	0.19015 mL	0.16381 mL	0.15000 mL	3.045	0.00047	0.00116	0.00068	10.0 s
44:36.3	Data point 42	2.20002 mL	0.19015 mL	0.16766 mL	0.15000 mL	3.275	0.00012	0.00005	0.00083	10.0 s
45:11.8	Data point 43	2.20002 mL	0.19015 mL	0.17027 mL	0.15000 mL	3.459	-0.00226	0.43409	0.00017	10.0 s
45:47.3	Data point 44	2.20002 mL	0.19015 mL	0.17222 mL	0.15000 mL	3.620	-0.01083	0.78989	0.00060	10.0 s
46:33.1	Data point 45	2.20002 mL	0.19015 mL	0.17404 mL	0.15000 mL	3.813	0.01106	0.77170	0.00062	10.0 s
47:24.1	Data point 46	2.20002 mL	0.19015 mL	0.17568 mL	0.15000 mL	4.007	-0.00395	0.53793	0.00027	10.0 s
48:15.0	Data point 47	2.20002 mL	0.19015 mL	0.17730 mL	0.15000 mL	4.193	-0.00655	0.22705	0.00068	10.0 s
49:06.0	Data point 48	2.20002 mL	0.19015 mL	0.17916 mL	0.15000 mL	4.376	0.00748	0.59754	0.00048	10.0 s
49:57.1	Data point 49	2.20002 mL	0.19015 mL	0.18123 mL	0.15000 mL	4.555	0.00753	0.36418	0.00062	10.0 s
50:42.9	Data point 50	2.20002 mL	0.19015 mL	0.18297 mL	0.15000 mL	4.737	-0.00461	0.27683	0.00043	10.0 s
51:18.3	Data point 51	2.20002 mL	0.19015 mL	0.18490 mL	0.15000 mL	4.999	-0.00646	0.54035	0.00043	10.5 s
51:59.5	Data point 52	2.20002 mL	0.19015 mL	0.18610 mL	0.15000 mL	5.180	-0.00205	0.01692	0.00078	10.0 s
52:45.2	Data point 53	2.20002 mL	0.19015 mL	0.18728 mL	0.15000 mL	5.395	0.00304	0.03920	0.00076	10.0 s
53:20.6	Data point 54	2.20002 mL	0.19015 mL	0.18808 mL	0.15000 mL	5.608	-0.01570	0.82199	0.00086	11.0 s
53:57.1	Data point 55	2.20002 mL	0.19015 mL	0.18869 mL	0.15000 mL	5.827	-0.01657	0.86910	0.00088	10.5 s
54:33.0	Data point 56	2.20002 mL	0.19015 mL	0.18914 mL	0.15000 mL	6.061	-0.01364	0.47158	0.00098	11.5 s
55:09.9	Data point 57	2.20002 mL	0.19015 mL	0.18944 mL	0.15000 mL	6.322	-0.01837	0.84621	0.00099	16.0 s
55:56.4	Data point 58	2.20002 mL	0.19015 mL	0.18965 mL	0.15000 mL	6.525	-0.01620	0.78360	0.00090	15.0 s
56:42.0	Data point 59	2.20002 mL	0.19015 mL	0.18979 mL	0.15000 mL	6.710	-0.01910	0.93669	0.00097	31.0 s
57:38.4	Data point 60	2.20002 mL	0.19015 mL	0.18989 mL	0.15000 mL	7.095	-0.01967	0.99319	0.00097	59.0 s
59:08.1	Data point 61	2.20002 mL	0.19015 mL	0.18998 mL	0.15000 mL	7.531	-0.03741	0.97375	0.00187	Timed out at 59.5 s
1:00:33.4	Data point 62	2.20002 mL	0.19015 mL	0.19001 mL	0.15000 mL	7.625	-0.01967	0.98081	0.00098	53.5 s
1:02:02.7	Data point 63	2.20002 mL	0.19015 mL	0.19007 mL	0.15000 mL	8.014	-0.01881	0.97922	0.00094	58.0 s
1:03:36.4	Data point 64	2.20002 mL	0.19015 mL	0.19015 mL	0.15000 mL	8.332	-0.01820	0.91738	0.00094	45.0 s
1:05:02.3	Data point 65	2.20002 mL	0.19015 mL	0.19024 mL	0.15000 mL	8.633	-0.01854	0.84927	0.00099	18.0 s
1:06:01.1	Data point 66	2.20002 mL	0.19015 mL	0.19038 mL	0.15000 mL	8.886	-0.01878	0.92878	0.00096	21.5 s
1:07:03.5	Data point 67	2.20002 mL	0.19015 mL	0.19052 mL	0.15000 mL	9.109	-0.01850	0.95816	0.00093	15.0 s
1:07:54.1	Data point 68	2.20002 mL	0.19015 mL	0.19069 mL	0.15000 mL	9.310	-0.01772	0.81325	0.00097	10.5 s
1:08:45.4	Data point 69	2.20002 mL	0.19015 mL	0.19095 mL	0.15000 mL	9.509	-0.01583	0.65574	0.00097	17.0 s
1:09:33.1	Data point 70	2.20002 mL	0.19015 mL	0.19130 mL	0.15000 mL	9.756	-0.01460	0.55168	0.00097	16.5 s
1:10:30.5	Data point 71	2.20002 mL	0.19015 mL	0.19172 mL	0.15000 mL	9.948	-0.00681	0.21656	0.00072	10.0 s
1:11:11.1	Data point 72	2.20002 mL	0.19015 mL	0.19191 mL	0.15000 mL	10.017	0.00087	0.01530	0.00035	10.0 s
1:12:27.4	Data point 73	2.20002 mL	0.29403 mL	0.19191 mL	0.45000 mL	1.972	-0.01003	0.70683	0.00059	10.0 s
1:13:13.9	Data point 74	2.20002 mL	0.29403 mL	0.21997 mL	0.45000 mL	2.175	0.00579	0.71483	0.00034	10.5 s
1:13:50.3	Data point 75	2.20002 mL	0.29403 mL	0.23942 mL	0.45000 mL	2.398	-0.00050	0.00121	0.00071	10.0 s
1:14:26.0	Data point 76	2.20002 mL	0.29403 mL	0.25212 mL	0.45000 mL	2.626	-0.01002	0.42775	0.00076	10.0 s
1:15:01.6	Data point 77	2.20002 mL	0.29403 mL	0.26056 mL	0.45000 mL	2.826	-0.00389	0.08255	0.00067	10.0 s
1:15:37.2	Data point 78	2.20002 mL	0.29403 mL	0.26653 mL	0.45000 mL	3.025	0.01417	0.79174	0.00079	10.0 s
1:16:12.6	Data point 79	2.20002 mL	0.29403 mL	0.27081 mL	0.45000 mL	3.243	0.00428	0.28164	0.00040	10.0 s
1:16:48.2	Data point 80	2.20002 mL	0.29403 mL	0.27382 mL	0.45000 mL	3.430	0.00870	0.54657	0.00058	10.5 s
1:17:24.2	Data point 81	2.20002 mL	0.29403 mL	0.27613 mL	0.45000 mL	3.577	-0.01656	0.72331	0.00096	15.0 s
1:18:20.2	Data point 82	2.20002 mL	0.29403 mL	0.27858 mL	0.45000 mL	3.754	0.00239	0.04126	0.00058	10.0 s
1:19:11.2	Data point 83	2.20002 mL	0.29403 mL	0.28074 mL	0.45000 mL	3.931	-0.00851	0.21217	0.00091	10.0 s
1:20:02.2	Data point 84	2.20002 mL	0.29403 mL	0.28311 mL	0.45000 mL	4.112	0.00633	0.50236	0.00044	10.0 s
1:20:53.2	Data point 85	2.20002 mL	0.29403 mL	0.28530 mL	0.45000 mL	4.288	0.00616	0.42147	0.00047	10.0 s
1:21:39.1	Data point 86	2.20002 mL	0.29403 mL	0.28716 mL	0.45000 mL	4.468	0.00653	0.41686	0.00050	10.5 s
1:22:15.1	Data point 87	2.20002 mL	0.29403 mL	0.28920 mL	0.45000 mL	4.750	-0.01024	0.56608	0.00067	10.5 s
1:22:56.2	Data point 88	2.20002 mL	0.29403 mL	0.29033 mL	0.45000 mL	4.921	-0.00504	0.30494	0.00045	10.5 s
1:23:32.1	Data point 89	2.20002 mL	0.29403 mL	0.29128 mL	0.45000 mL	5.107	-0.00661	0.13487	0.00089	10.0 s
1:24:07.6	Data point 90	2.20002 mL	0.29403 mL	0.29207 mL	0.45000 mL	5.317	-0.00338	0.02804	0.00100	17.0 s
1:24:50.0	Data point 91	2.20002 mL	0.29403 mL	0.29269 mL	0.45000 mL	5.549	-0.00970	0.38066	0.00078	11.0 s
1:25:26.4	Data point 92	2.20002 mL	0.29403 mL	0.29311 mL	0.45000 mL	5.831	-0.01048	0.30330	0.00094	12.5 s
1:26:04.3	Data point 93	2.20002 mL	0.29403 mL	0.29337 mL	0.45000 mL	6.110	-0.01816	0.86837	0.00096	31.0 s

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Events (continued)

Time	Event	Water	Acid	Base	Octanol	pH	dpH/dt	pH R-squared	pH SD	dpH/dt time
1:27:00.8	Data point 94	2.20002 mL	0.29403 mL	0.29353 mL	0.45000 mL	6.366	-0.01843	0.94543	0.00094	42.0 s
1:28:13.4	Data point 95	2.20002 mL	0.29403 mL	0.29370 mL	0.45000 mL	6.669	-0.01870	0.98301	0.00093	56.0 s
1:29:40.0	Data point 96	2.20002 mL	0.29403 mL	0.29379 mL	0.45000 mL	6.935	-0.02391	0.96793	0.00120	Timed out at 59.5 s
1:31:10.7	Data point 97	2.20002 mL	0.29403 mL	0.29386 mL	0.45000 mL	7.222	-0.03766	0.98462	0.00187	Timed out at 59.5 s
1:32:41.3	Data point 98	2.20002 mL	0.29403 mL	0.29403 mL	0.45000 mL	8.270	-0.03076	0.99007	0.00153	Timed out at 59.5 s
1:34:16.9	Data point 99	2.20002 mL	0.29403 mL	0.29417 mL	0.45000 mL	8.626	-0.01455	0.55806	0.00096	17.5 s
1:35:10.1	Data point 100	2.20002 mL	0.29403 mL	0.29433 mL	0.45000 mL	8.885	0.00677	0.11530	0.00099	21.5 s
1:36:12.4	Data point 101	2.20002 mL	0.29403 mL	0.29454 mL	0.45000 mL	9.111	-0.00911	0.28833	0.00084	11.5 s
1:36:59.8	Data point 102	2.20002 mL	0.29403 mL	0.29473 mL	0.45000 mL	9.302	-0.01144	0.38459	0.00091	12.0 s
1:37:52.6	Data point 103	2.20002 mL	0.29403 mL	0.29501 mL	0.45000 mL	9.516	-0.01706	0.74556	0.00098	11.0 s
1:38:44.4	Data point 104	2.20002 mL	0.29403 mL	0.29534 mL	0.45000 mL	9.718	-0.01826	0.87768	0.00096	10.0 s
1:39:35.4	Data point 105	2.20002 mL	0.29403 mL	0.29574 mL	0.45000 mL	9.922	-0.00385	0.15864	0.00048	10.5 s
1:40:16.4	Data point 106	2.20002 mL	0.29403 mL	0.29598 mL	0.45000 mL	10.023	-0.00776	0.63643	0.00048	10.5 s
1:40:36.1	Assay volumes	2.20002 mL	0.29403 mL	0.29598 mL	0.45000 mL					

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings

Setting	Value	Original Value	Date/Time changed	Imported from
General Settings				
Analyst name	Pion			
Standard Experiment Settings				
Number of titrations	3			
Minimum pH	2.000			
Maximum pH	10.000			
pH step between points of	0.200			
Minimum titrant addition	0.00002 mL			
Maximum titrant addition	0.10000 mL			
Argon flow rate	100%			
Start titration using	Cautious pH adjust			
Advanced General Settings				
Detect turbidity using	None			
Collect turbidity sensor data	No			
Collect UV spectra	No			
Stir after titrant addition for	5 seconds			
For titrant addition, stir at	10%			
Titrant Pre-Dose				
Titrant pre-dose	None			
Assay Medium				
ISA water volume	2.20 mL			
Water added	Automatic			
Partition solvent type	Octanol			
Partition volume	0.050 mL			
Partition solvent added	Automatic			
After partition addition, stir for	1 seconds			
Sample Sonication				
Sonicate	Yes			
Adjust pH for sonication	No			
Sonicate for	300 seconds			
After sonication stir for	5 seconds			
Sample Dissolution				
Perform a dissolution stage	Yes			
Adjust and hold pH for dissolution	To start pH			
Stir to dissolve for	120 seconds			
For dissolution, stir at	10%			
Carbonate purge				
Perform a carbonate purge	No			
Temperature Control				
Wait for temperature	Yes			
Required start temperature	25.0°C			
Acceptable deviation	0.5°C			
Time to wait	60 seconds			
Stir speed of	50%			
Titration 1				
Titrate from	Low to high pH			
Adjust to start pH	Yes			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	50%			
Titration 2				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.100 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	55%			

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Assay Settings (continued)

Setting	Value	Original Value	Date/Time changed	Imported from
Titration 3				
Titrate from	Low to high pH			
Add additional water	0.00 mL			
Additional partition solvent volume	0.300 mL			
Additional partition solvent added	Automatic			
After pH adjust stir for	30 seconds			
Stir to allow partitioning for	15 seconds			
Stirrer speed for partitioning	60%			
Data Point Stability				
Stir during data point collection	No			
Delay before data point collection	0 seconds			
Number of points to average	20 points			
Time interval between points	0.50 seconds			
Required maximum standard deviation	0.00100 dpH/dt			
Stability timeout after	60 seconds			

Calibration Settings

Setting	Value	Date/Time changed	Imported from
Four-Plus alpha	0.130	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus S	0.9970	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jH	0.8	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
Four-Plus jOH	-0.4	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r
Base concentration factor	1.000	2/28/2018 1:10:47 AM	C:\Sirius_T3\KOH18B27.t3r
Acid concentration factor	0.994	2/28/2018 1:10:47 AM	C:\Sirius_T3\HCl18B27.t3r

Instrument Settings

Setting	Value	Batch Id	Install date
Instrument owner	Merck		
Instrument ID	T312060		
Instrument type	T3 Simulator		
Software version	1.1.3.0		
Dispenser module		T3DM1200361	3/31/2009 5:24:52 AM
Dispenser 0	Water		3/31/2009 5:25:05 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Water (0.15 M KCl)	02-06-2018	2/27/2018 10:05:59 AM
Dispenser 2	Acid		3/31/2009 5:25:11 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Acid (0.5 M HCl)	02-27-2018	2/27/2018 10:27:22 AM
Dispenser 1	Base		3/31/2009 5:25:21 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Base (0.5 M KOH)	9/22/2017	2/27/2018 10:21:22 AM
Dispenser 5	Cosolvent		3/31/2009 5:26:24 AM
Syringe volume	2.5 mL		
Firmware version	1.2.1(r2)		
Distribution valve 5	Distribution Valve		3/31/2009 5:28:19 AM
Firmware version	1.1.3		
Port A	Methanol (80%, 0.15 M KCl)	09-26-17	2/7/2018 9:42:01 AM
Port B	Cyclohexane	11-01-17	2/27/2018 10:37:57 AM
Dispenser 3	Buffer		8/3/2010 5:05:16 AM
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Dodecane	2018/01/31	1/31/2018 12:26:26 PM
Dispenser 6	Octanol		10/22/2010 10:52:43 AM

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Syringe volume	0.5 mL		
Firmware version	1.2.1(r2)		
Titrant	Octanol	01-31-2018	2/27/2018 9:59:35 AM
Titrator		T3TM1200161	3/31/2009 5:24:17 AM
Horizontal axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Probe I/O firmware version	1.1.1		
Electrode	T3 Electrode	T3E0923	1/23/2018 2:01:00 PM
E0 calibration	+2.60 mV		2/28/2018 1:11:15 AM
Filling solution	3M KCl	KCL097	2/27/2018 9:49:43 AM
Liquids			
Wash 1	50% IPA:50% Water		2/27/2018 9:49:58 AM
Wash 2	0.5% Trition X-100 in H20		2/27/2018 9:50:01 AM
Buffer position 1	pH7 Wash		2/27/2018 9:50:04 AM
Buffer position 2	pH 7		2/27/2018 9:50:06 AM
Storage position			2/27/2018 9:55:12 AM
Wash water	9.1e+003 mL	02-27-2018	2/27/2018 9:54:39 AM
Waste	6.3e+003 mL		11/28/2017 10:36:29 AM
Temperature controller			8/5/2010 6:35:13 AM
Turbidity detector			3/31/2009 5:24:45 AM
Spectrometer		074811	11/23/2010 11:22:28 AM
Dip probe		10196	
Wavelength coefficient A0	183.333		
Wavelength coefficient A1	2.21568		
Wavelength coefficient A2	-0.000289308		
Total lamp lit time	110:52:56		11/23/2010 11:22:28 AM
Calibrated on	2/27/2018 10:40:38 AM		
Integration time	40		
Scans averaged	10		
Autoloader		T3AL1200345	11/10/2015 9:34:13 AM
Left-right axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Front-back axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Vertical axis firmware version	1.17 AI1DI2DO2 Stepper 2		
Chassis I/O firmware version	1.11 AI1DI0DO4 Norgren I/O		
Configuration			
Alternate titration position	Titration position		
Alternate reference position	Reference position		
Maximum standard vial volume	3.50 mL		
Maximum alternate vial volume	25.00 mL		
Automatic action idle period	5 minute(s)		
Titrant tube volume	1.3 mL		
Syringe flush count	3.50		
Flowing wash pump volume	20.0 mL		
Flowing wash stir duration	5 s		
Flowing wash stir speed	30%		
Solvent wash stir duration	5 s		
Solvent wash stir speed	30%		
Surfactant wash stir duration	5 s		
Surfactant wash stir speed	30%		
E0 calibration minimum number of points	10		
E0 calibration maximum standard deviation	0.01500		
E0 calibration timeout period	60 s		
E0 calibration stir duration	5 s		
E0 calibration preparation stir speed	30%		
E0 calibration buffer wash stir duration	5 s		
E0 calibration buffer wash stir speed	30%		
E0 calibration reading stir speed	0%		

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Instrument Settings (continued)

Setting	Value	Batch Id	Install date
Spectrometer calibration stir duration	5 s		
Spectrometer calibration stir speed	30%		
Spectrometer calibration wash pump volume	20.0 mL		
Spectrometer calibration wash stir duration	5 s		
Spectrometer calibration wash stir speed	30%		
Overhead dispense height	10000		

Refinement Settings

Setting	Value	Default value
Turbidity detection method	None	None
Turbidity wavelength to assess	500.0 nm	500.0 nm
Turbidity maximum absorbance	0.100	0.100
Turbidity probe threshold	50.00	50.00

Experiment Log

[2:37] Air gap created for Water (0.15 M KCl)
[2:37] Air gap created for Acid (0.5 M HCl)
[2:38] Air gap created for Base (0.5 M KOH)
[2:38] Air gap released for Water (0.15 M KCl)
[2:42] Titrator arm moved over Titration position
[2:42] Titration 1 of 3
[2:42] Adding initial titrants
[2:42] Automatically add 2.20000 mL of water
[3:19] Dispensed 2.200024 mL of Water (0.15 M KCl)
[3:23] Titrator arm moved over Drain
[9:05] Titrator arm moved to Titration position
[9:05] Argon flow rate set to 100
[9:05] Stirrer speed set to 10
[9:10] Automatically add 0.05000 mL of Octanol
[9:11] Dispensed 0.050000 mL of Octanol
[9:12] Initial pH = 6.77
[9:12] Iterative adjust 6.77 -> 2.00
[9:12] pH 6.77 -> 2.00
[9:15] Air gap released for Acid (0.5 M HCl)
[9:15] Dispensed 0.091745 mL of Acid (0.5 M HCl)
[9:21] Holding pH 2.00
[11:21] Stirrer speed set to 0
[11:21] Stirrer speed set to 50
[11:21] Iterative adjust 1.95 -> 2.00
[11:21] pH 1.95 -> 2.00
[11:21] Air gap released for Base (0.5 M KOH)
[11:22] Dispensed 0.008843 mL of Base (0.5 M KOH)
[12:13] Stirrer speed set to 0
[12:23] Datapoint id 1 collected
[12:23] Stirrer speed set to 50
[12:28] pH 2.01 -> 2.21
[12:28] Using cautious pH adjust
[12:28] Dispensed 0.012112 mL of Base (0.5 M KOH)
[12:33] Stepping pH = 2.10
[12:34] Dispensed 0.008631 mL of Base (0.5 M KOH)
[12:39] Stepping pH = 2.18
[12:39] Dispensed 0.002281 mL of Base (0.5 M KOH)
[12:44] Stepping pH = 2.21
[12:59] Stirrer speed set to 0
[13:09] Datapoint id 2 collected
[13:09] Charge balance equation is out by 4.9%
[13:09] Stirrer speed set to 50

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[13:14] pH 2.22 -> 2.42
[13:14] Using charge balance adjust
[13:15] Dispensed 0.015734 mL of Base (0.5 M KOH)
[13:35] Stirrer speed set to 0
[13:45] Datapoint id 3 collected
[13:45] Charge balance equation is out by 9.6%
[13:45] Stirrer speed set to 50
[13:50] pH 2.44 -> 2.64
[13:50] Using charge balance adjust
[13:51] Dispensed 0.010278 mL of Base (0.5 M KOH)
[14:11] Stirrer speed set to 0
[14:21] Datapoint id 4 collected
[14:21] Charge balance equation is out by 6.7%
[14:21] Stirrer speed set to 50
[14:26] pH 2.66 -> 2.86
[14:26] Using charge balance adjust
[14:26] Dispensed 0.007032 mL of Base (0.5 M KOH)
[14:47] Stirrer speed set to 0
[14:57] Datapoint id 5 collected
[14:57] Charge balance equation is out by 19.7%
[14:57] Stirrer speed set to 50
[15:02] pH 2.91 -> 3.11
[15:02] Using cautious pH adjust
[15:02] Dispensed 0.002305 mL of Base (0.5 M KOH)
[15:07] Stepping pH = 2.99
[15:07] Dispensed 0.002023 mL of Base (0.5 M KOH)
[15:12] Stepping pH = 3.08
[15:12] Dispensed 0.000517 mL of Base (0.5 M KOH)
[15:17] Stepping pH = 3.11
[15:32] Stirrer speed set to 0
[15:42] Datapoint id 6 collected
[15:42] Charge balance equation is out by -4.8%
[15:42] Stirrer speed set to 50
[15:48] pH 3.12 -> 3.32
[15:48] Using charge balance adjust
[15:48] Dispensed 0.003246 mL of Base (0.5 M KOH)
[16:08] Stirrer speed set to 0
[16:18] Datapoint id 7 collected
[16:18] Charge balance equation is out by 13.6%
[16:18] Stirrer speed set to 50
[16:23] pH 3.35 -> 3.55
[16:23] Using charge balance adjust
[16:23] Dispensed 0.002164 mL of Base (0.5 M KOH)
[16:43] Stirrer speed set to 0
[16:53] Datapoint id 8 collected
[16:53] Charge balance equation is out by 3.6%
[16:53] Stirrer speed set to 50
[16:59] pH 3.56 -> 3.76
[16:59] Using charge balance adjust
[16:59] Dispensed 0.001529 mL of Base (0.5 M KOH)
[17:19] Stirrer speed set to 0
[17:29] Datapoint id 9 collected
[17:29] Charge balance equation is out by -14.3%
[17:29] Stirrer speed set to 50
[17:34] pH 3.75 -> 3.95
[17:34] Using charge balance adjust
[17:34] Dispensed 0.001176 mL of Base (0.5 M KOH)
[17:54] Stirrer speed set to 0
[18:04] Datapoint id 10 collected

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**
Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[18:04] Charge balance equation is out by -20.3%
[18:04] Stirrer speed set to 50
[18:09] pH 3.92 -> 4.12
[18:09] Using cautious pH adjust
[18:10] Dispensed 0.000517 mL of Base (0.5 M KOH)
[18:15] Stepping pH = 4.00
[18:15] Dispensed 0.000470 mL of Base (0.5 M KOH)
[18:20] Stepping pH = 4.09
[18:20] Dispensed 0.000118 mL of Base (0.5 M KOH)
[18:25] Stepping pH = 4.10
[18:25] Dispensed 0.000118 mL of Base (0.5 M KOH)
[18:30] Stepping pH = 4.12
[18:45] Stirrer speed set to 0
[18:55] Datapoint id 11 collected
[18:55] Charge balance equation is out by -18.7%
[18:55] Stirrer speed set to 50
[19:00] pH 4.13 -> 4.33
[19:00] Using cautious pH adjust
[19:00] Dispensed 0.000517 mL of Base (0.5 M KOH)
[19:05] Stepping pH = 4.26
[19:06] Dispensed 0.000259 mL of Base (0.5 M KOH)
[19:11] Stepping pH = 4.31
[19:11] Dispensed 0.000071 mL of Base (0.5 M KOH)
[19:16] Stepping pH = 4.32
[19:16] Dispensed 0.000141 mL of Base (0.5 M KOH)
[19:21] Stepping pH = 4.35
[19:36] Stirrer speed set to 0
[19:47] Datapoint id 12 collected
[19:47] Charge balance equation is out by 3.7%
[19:47] Stirrer speed set to 50
[19:52] pH 4.35 -> 4.55
[19:52] Using charge balance adjust
[19:52] Dispensed 0.001152 mL of Base (0.5 M KOH)
[20:12] Stirrer speed set to 0
[20:22] Datapoint id 13 collected
[20:22] Charge balance equation is out by 17.7%
[20:22] Stirrer speed set to 50
[20:27] pH 4.59 -> 4.79
[20:27] Using cautious pH adjust
[20:27] Dispensed 0.000729 mL of Base (0.5 M KOH)
[20:32] Stepping pH = 4.71
[20:33] Dispensed 0.000400 mL of Base (0.5 M KOH)
[20:38] Stepping pH = 4.77
[20:38] Dispensed 0.000094 mL of Base (0.5 M KOH)
[20:43] Stepping pH = 4.77
[20:43] Dispensed 0.000094 mL of Base (0.5 M KOH)
[20:48] Stepping pH = 4.79
[21:03] Stirrer speed set to 0
[21:14] Datapoint id 14 collected
[21:14] Charge balance equation is out by 8.9%
[21:14] Stirrer speed set to 50
[21:19] pH 4.78 -> 4.98
[21:19] Using charge balance adjust
[21:19] Dispensed 0.001740 mL of Base (0.5 M KOH)
[21:39] Stirrer speed set to 0
[21:50] Datapoint id 15 collected
[21:50] Charge balance equation is out by 16.6%
[21:50] Stirrer speed set to 50
[21:55] pH 5.02 -> 5.22

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[21:55] Using cautious pH adjust
[21:55] Dispensed 0.000988 mL of Base (0.5 M KOH)
[22:00] Stepping pH = 5.14
[22:00] Dispensed 0.000494 mL of Base (0.5 M KOH)
[22:05] Stepping pH = 5.20
[22:05] Dispensed 0.000188 mL of Base (0.5 M KOH)
[22:10] Stepping pH = 5.21
[22:25] Stirrer speed set to 0
[22:35] Datapoint id 16 collected
[22:35] Charge balance equation is out by 15.1%
[22:35] Stirrer speed set to 50
[22:40] pH 5.20 -> 5.40
[22:40] Using cautious pH adjust
[22:41] Dispensed 0.001011 mL of Base (0.5 M KOH)
[22:46] Stepping pH = 5.32
[22:46] Dispensed 0.000517 mL of Base (0.5 M KOH)
[22:51] Stepping pH = 5.39
[22:51] Dispensed 0.000118 mL of Base (0.5 M KOH)
[22:56] Stepping pH = 5.39
[22:56] Dispensed 0.000118 mL of Base (0.5 M KOH)
[23:01] Stepping pH = 5.41
[23:16] Stirrer speed set to 0
[23:27] Datapoint id 17 collected
[23:27] Charge balance equation is out by 12.5%
[23:27] Stirrer speed set to 50
[23:32] pH 5.40 -> 5.60
[23:32] Using charge balance adjust
[23:32] Dispensed 0.001858 mL of Base (0.5 M KOH)
[23:52] Stirrer speed set to 0
[24:03] Datapoint id 18 collected
[24:03] Charge balance equation is out by 72.8%
[24:03] Stirrer speed set to 50
[24:08] pH 5.75 -> 5.95
[24:08] Using cautious pH adjust
[24:08] Dispensed 0.000659 mL of Base (0.5 M KOH)
[24:13] Stepping pH = 5.93
[24:13] Dispensed 0.000071 mL of Base (0.5 M KOH)
[24:18] Stepping pH = 5.93
[24:18] Dispensed 0.000118 mL of Base (0.5 M KOH)
[24:23] Stepping pH = 5.97
[24:38] Stirrer speed set to 0
[24:49] Datapoint id 19 collected
[24:49] Charge balance equation is out by 34.9%
[24:49] Stirrer speed set to 50
[24:54] pH 5.97 -> 6.17
[24:54] Using cautious pH adjust
[24:54] Dispensed 0.000494 mL of Base (0.5 M KOH)
[24:59] Stepping pH = 6.20
[25:14] Stirrer speed set to 0
[25:24] Datapoint id 20 collected
[25:24] Charge balance equation is out by 50.0%
[25:24] Stirrer speed set to 50
[25:29] pH 6.20 -> 6.40
[25:29] Using cautious pH adjust
[25:29] Dispensed 0.000329 mL of Base (0.5 M KOH)
[25:34] Stepping pH = 6.42
[25:49] Stirrer speed set to 0
[26:00] Datapoint id 21 collected
[26:00] Charge balance equation is out by 50.0%

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[26:00] Stirrer speed set to 50
[26:05] pH 6.42 -> 6.62
[26:05] Using cautious pH adjust
[26:05] Dispensed 0.000212 mL of Base (0.5 M KOH)
[26:10] Stepping pH = 6.60
[26:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:15] Stepping pH = 6.61
[26:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[26:20] Stepping pH = 6.62
[26:36] Stirrer speed set to 0
[26:46] Datapoint id 22 collected
[26:46] Charge balance equation is out by 37.9%
[26:46] Stirrer speed set to 50
[26:51] pH 6.62 -> 6.82
[26:51] Using cautious pH adjust
[26:51] Dispensed 0.000141 mL of Base (0.5 M KOH)
[26:56] Stepping pH = 6.84
[27:11] Stirrer speed set to 0
[27:45] Datapoint id 23 collected
[27:45] Charge balance equation is out by 50.0%
[27:45] Stirrer speed set to 50
[27:51] pH 6.85 -> 7.05
[27:51] Using cautious pH adjust
[27:51] Dispensed 0.000094 mL of Base (0.5 M KOH)
[27:56] Stepping pH = 7.02
[27:56] Dispensed 0.000024 mL of Base (0.5 M KOH)
[28:01] Stepping pH = 7.06
[28:16] Stirrer speed set to 0
[28:51] Datapoint id 24 collected
[28:51] Charge balance equation is out by 39.1%
[28:51] Stirrer speed set to 50
[28:56] pH 7.08 -> 7.28
[28:56] Using cautious pH adjust
[28:56] Dispensed 0.000047 mL of Base (0.5 M KOH)
[29:01] Stepping pH = 7.19
[29:01] Dispensed 0.000024 mL of Base (0.5 M KOH)
[29:07] Stepping pH = 7.28
[29:22] Stirrer speed set to 0
[30:11] Datapoint id 25 collected
[30:11] Charge balance equation is out by 23.6%
[30:11] Stirrer speed set to 50
[30:16] pH 7.30 -> 7.50
[30:16] Using cautious pH adjust
[30:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[30:21] Stepping pH = 7.31
[30:22] Dispensed 0.000094 mL of Base (0.5 M KOH)
[30:27] Stepping pH = 8.01
[30:42] Stirrer speed set to 0
[31:42] Datapoint id 26 collected
[31:42] Charge balance equation is out by -92.6%
[31:42] Stirrer speed set to 50
[31:47] pH 8.09 -> 8.29
[31:47] Using cautious pH adjust
[31:47] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:52] Stepping pH = 8.11
[31:52] Dispensed 0.000024 mL of Base (0.5 M KOH)
[31:57] Stepping pH = 8.18
[31:57] Dispensed 0.000024 mL of Base (0.5 M KOH)
[32:02] Stepping pH = 8.30

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[32:17] Stirrer speed set to 0
[33:00] Datapoint id 27 collected
[33:00] Charge balance equation is out by -279.3%
[33:00] Stirrer speed set to 50
[33:05] pH 8.36 -> 8.56
[33:05] Using cautious pH adjust
[33:05] Dispensed 0.000024 mL of Base (0.5 M KOH)
[33:10] Stepping pH = 8.38
[33:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[33:15] Stepping pH = 8.46
[33:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[33:21] Stepping pH = 8.56
[33:36] Stirrer speed set to 0
[34:15] Datapoint id 28 collected
[34:15] Charge balance equation is out by -251.0%
[34:15] Stirrer speed set to 50
[34:20] pH 8.60 -> 8.80
[34:20] Using cautious pH adjust
[34:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[34:25] Stepping pH = 8.62
[34:25] Dispensed 0.000047 mL of Base (0.5 M KOH)
[34:30] Stepping pH = 8.79
[34:30] Dispensed 0.000024 mL of Base (0.5 M KOH)
[34:35] Stepping pH = 8.85
[34:50] Stirrer speed set to 0
[35:11] Datapoint id 29 collected
[35:11] Charge balance equation is out by -177.5%
[35:11] Stirrer speed set to 50
[35:16] pH 8.86 -> 9.06
[35:16] Using cautious pH adjust
[35:17] Dispensed 0.000024 mL of Base (0.5 M KOH)
[35:22] Stepping pH = 8.87
[35:22] Dispensed 0.000071 mL of Base (0.5 M KOH)
[35:27] Stepping pH = 9.07
[35:42] Stirrer speed set to 0
[36:11] Datapoint id 30 collected
[36:11] Charge balance equation is out by -92.2%
[36:11] Stirrer speed set to 50
[36:16] pH 9.08 -> 9.28
[36:16] Using cautious pH adjust
[36:16] Dispensed 0.000047 mL of Base (0.5 M KOH)
[36:21] Stepping pH = 9.12
[36:21] Dispensed 0.000071 mL of Base (0.5 M KOH)
[36:26] Stepping pH = 9.27
[36:41] Stirrer speed set to 0
[36:58] Datapoint id 31 collected
[36:58] Charge balance equation is out by -49.9%
[36:58] Stirrer speed set to 50
[37:03] pH 9.28 -> 9.48
[37:03] Using cautious pH adjust
[37:03] Dispensed 0.000047 mL of Base (0.5 M KOH)
[37:08] Stepping pH = 9.30
[37:08] Dispensed 0.000141 mL of Base (0.5 M KOH)
[37:13] Stepping pH = 9.51
[37:28] Stirrer speed set to 0
[37:42] Datapoint id 32 collected
[37:42] Charge balance equation is out by -87.7%
[37:42] Stirrer speed set to 50
[37:47] pH 9.52 -> 9.72

Sample name: **M15_octanol**
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Experiment start time: **2/28/2018 1:10:47 AM**
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Instrument ID: **T312060**

Experiment Log (continued)

[37:47] Using cautious pH adjust
[37:47] Dispensed 0.000094 mL of Base (0.5 M KOH)
[37:52] Stepping pH = 9.58
[37:52] Dispensed 0.000118 mL of Base (0.5 M KOH)
[37:57] Stepping pH = 9.69
[37:58] Dispensed 0.000024 mL of Base (0.5 M KOH)
[38:03] Stepping pH = 9.70
[38:03] Dispensed 0.000024 mL of Base (0.5 M KOH)
[38:08] Stepping pH = 9.71
[38:23] Stirrer speed set to 0
[38:33] Datapoint id 33 collected
[38:33] Charge balance equation is out by -52.5%
[38:33] Stirrer speed set to 50
[38:39] pH 9.71 -> 9.91
[38:39] Using cautious pH adjust
[38:39] Dispensed 0.000118 mL of Base (0.5 M KOH)
[38:44] Stepping pH = 9.80
[38:44] Dispensed 0.000118 mL of Base (0.5 M KOH)
[38:49] Stepping pH = 9.88
[38:49] Dispensed 0.000047 mL of Base (0.5 M KOH)
[38:54] Stepping pH = 9.91
[39:09] Stirrer speed set to 0
[39:20] Datapoint id 34 collected
[39:20] Charge balance equation is out by -10.0%
[39:20] Stirrer speed set to 50
[39:25] pH 9.91 -> 10.05
[39:25] Using charge balance adjust
[39:25] Dispensed 0.000235 mL of Base (0.5 M KOH)
[39:45] Stirrer speed set to 0
[39:55] Datapoint id 35 collected
[39:55] Charge balance equation is out by -45.0%
[39:55] Titration 2 of 3
[39:55] Adding initial titrants
[39:55] Automatically add 0.10000 mL of Octanol
[39:58] Dispensed 0.100000 mL of Octanol
[39:58] Stirrer speed set to 10
[39:59] Stirrer speed set to 55
[39:59] Iterative adjust 10.03 -> 2.00
[39:59] pH 10.03 -> 2.00
[40:01] Dispensed 0.098401 mL of Acid (0.5 M HCl)
[40:51] Stirrer speed set to 0
[41:01] Datapoint id 36 collected
[41:01] Stirrer speed set to 55
[41:06] pH 1.97 -> 2.17
[41:06] Using cautious pH adjust
[41:07] Dispensed 0.014111 mL of Base (0.5 M KOH)
[41:12] Stepping pH = 2.07
[41:12] Dispensed 0.010278 mL of Base (0.5 M KOH)
[41:17] Stepping pH = 2.15
[41:18] Dispensed 0.002658 mL of Base (0.5 M KOH)
[41:23] Stepping pH = 2.18
[41:38] Stirrer speed set to 0
[41:48] Datapoint id 37 collected
[41:48] Charge balance equation is out by 4.2%
[41:48] Stirrer speed set to 55
[41:53] pH 2.19 -> 2.39
[41:53] Using charge balance adjust
[41:53] Dispensed 0.018062 mL of Base (0.5 M KOH)
[42:14] Stirrer speed set to 0

Sample name: **M15_octanol**
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Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[42:24] Datapoint id 38 collected
[42:24] Charge balance equation is out by 5.1%
[42:24] Stirrer speed set to 55
[42:29] pH 2.40 -> 2.60
[42:29] Using charge balance adjust
[42:29] Dispensed 0.011900 mL of Base (0.5 M KOH)
[42:49] Stirrer speed set to 0
[42:59] Datapoint id 39 collected
[42:59] Charge balance equation is out by 11.2%
[42:59] Stirrer speed set to 55
[43:05] pH 2.63 -> 2.83
[43:05] Using charge balance adjust
[43:05] Dispensed 0.007926 mL of Base (0.5 M KOH)
[43:25] Stirrer speed set to 0
[43:35] Datapoint id 40 collected
[43:35] Charge balance equation is out by 3.5%
[43:35] Stirrer speed set to 55
[43:40] pH 2.84 -> 3.04
[43:40] Using charge balance adjust
[43:40] Dispensed 0.005503 mL of Base (0.5 M KOH)
[44:01] Stirrer speed set to 0
[44:11] Datapoint id 41 collected
[44:11] Charge balance equation is out by 1.6%
[44:11] Stirrer speed set to 55
[44:16] pH 3.05 -> 3.25
[44:16] Using charge balance adjust
[44:16] Dispensed 0.003857 mL of Base (0.5 M KOH)
[44:36] Stirrer speed set to 0
[44:46] Datapoint id 42 collected
[44:46] Charge balance equation is out by 10.8%
[44:46] Stirrer speed set to 55
[44:51] pH 3.28 -> 3.48
[44:51] Using charge balance adjust
[44:51] Dispensed 0.002611 mL of Base (0.5 M KOH)
[45:12] Stirrer speed set to 0
[45:22] Datapoint id 43 collected
[45:22] Charge balance equation is out by -10.7%
[45:22] Stirrer speed set to 55
[45:27] pH 3.46 -> 3.66
[45:27] Using charge balance adjust
[45:27] Dispensed 0.001952 mL of Base (0.5 M KOH)
[45:47] Stirrer speed set to 0
[45:57] Datapoint id 44 collected
[45:57] Charge balance equation is out by -21.3%
[45:57] Stirrer speed set to 55
[46:02] pH 3.63 -> 3.83
[46:02] Using cautious pH adjust
[46:02] Dispensed 0.000776 mL of Base (0.5 M KOH)
[46:07] Stepping pH = 3.70
[46:07] Dispensed 0.000729 mL of Base (0.5 M KOH)
[46:13] Stepping pH = 3.78
[46:13] Dispensed 0.000306 mL of Base (0.5 M KOH)
[46:18] Stepping pH = 3.82
[46:33] Stirrer speed set to 0
[46:43] Datapoint id 45 collected
[46:43] Charge balance equation is out by -17.3%
[46:43] Stirrer speed set to 55
[46:48] pH 3.82 -> 4.02
[46:48] Using cautious pH adjust

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
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Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[46:48] Dispensed 0.000659 mL of Base (0.5 M KOH)
[46:53] Stepping pH = 3.90
[46:53] Dispensed 0.000588 mL of Base (0.5 M KOH)
[46:58] Stepping pH = 3.98
[46:58] Dispensed 0.000282 mL of Base (0.5 M KOH)
[47:04] Stepping pH = 4.01
[47:04] Dispensed 0.000118 mL of Base (0.5 M KOH)
[47:09] Stepping pH = 4.02
[47:24] Stirrer speed set to 0
[47:34] Datapoint id 46 collected
[47:34] Charge balance equation is out by -25.1%
[47:34] Stirrer speed set to 55
[47:39] pH 4.01 -> 4.21
[47:39] Using cautious pH adjust
[47:39] Dispensed 0.000611 mL of Base (0.5 M KOH)
[47:44] Stepping pH = 4.09
[47:44] Dispensed 0.000588 mL of Base (0.5 M KOH)
[47:49] Stepping pH = 4.16
[47:49] Dispensed 0.000306 mL of Base (0.5 M KOH)
[47:55] Stepping pH = 4.20
[47:55] Dispensed 0.000118 mL of Base (0.5 M KOH)
[48:00] Stepping pH = 4.20
[48:15] Stirrer speed set to 0
[48:25] Datapoint id 47 collected
[48:25] Charge balance equation is out by -30.8%
[48:25] Stirrer speed set to 55
[48:30] pH 4.20 -> 4.40
[48:30] Using cautious pH adjust
[48:30] Dispensed 0.000659 mL of Base (0.5 M KOH)
[48:35] Stepping pH = 4.27
[48:35] Dispensed 0.000682 mL of Base (0.5 M KOH)
[48:40] Stepping pH = 4.34
[48:40] Dispensed 0.000376 mL of Base (0.5 M KOH)
[48:46] Stepping pH = 4.38
[48:46] Dispensed 0.000141 mL of Base (0.5 M KOH)
[48:51] Stepping pH = 4.39
[49:06] Stirrer speed set to 0
[49:16] Datapoint id 48 collected
[49:16] Charge balance equation is out by -41.1%
[49:16] Stirrer speed set to 55
[49:21] pH 4.38 -> 4.58
[49:21] Using cautious pH adjust
[49:21] Dispensed 0.000753 mL of Base (0.5 M KOH)
[49:26] Stepping pH = 4.45
[49:26] Dispensed 0.000800 mL of Base (0.5 M KOH)
[49:31] Stepping pH = 4.54
[49:32] Dispensed 0.000353 mL of Base (0.5 M KOH)
[49:37] Stepping pH = 4.56
[49:37] Dispensed 0.000165 mL of Base (0.5 M KOH)
[49:42] Stepping pH = 4.57
[49:57] Stirrer speed set to 0
[50:07] Datapoint id 49 collected
[50:07] Charge balance equation is out by -36.8%
[50:07] Stirrer speed set to 55
[50:12] pH 4.56 -> 4.76
[50:12] Using cautious pH adjust
[50:12] Dispensed 0.000870 mL of Base (0.5 M KOH)
[50:17] Stepping pH = 4.66
[50:17] Dispensed 0.000659 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
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Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[50:22] Stepping pH = 4.74
[50:22] Dispensed 0.000212 mL of Base (0.5 M KOH)
[50:28] Stepping pH = 4.75
[50:43] Stirrer speed set to 0
[50:53] Datapoint id 50 collected
[50:53] Charge balance equation is out by 0.1%
[50:53] Stirrer speed set to 55
[50:58] pH 4.74 -> 4.94
[50:58] Using charge balance adjust
[50:58] Dispensed 0.001929 mL of Base (0.5 M KOH)
[51:18] Stirrer speed set to 0
[51:29] Datapoint id 51 collected
[51:29] Charge balance equation is out by 29.5%
[51:29] Stirrer speed set to 55
[51:34] pH 5.00 -> 5.20
[51:34] Using cautious pH adjust
[51:34] Dispensed 0.001011 mL of Base (0.5 M KOH)
[51:39] Stepping pH = 5.17
[51:39] Dispensed 0.000188 mL of Base (0.5 M KOH)
[51:44] Stepping pH = 5.20
[51:59] Stirrer speed set to 0
[52:09] Datapoint id 52 collected
[52:09] Charge balance equation is out by 41.1%
[52:09] Stirrer speed set to 55
[52:14] pH 5.19 -> 5.39
[52:14] Using cautious pH adjust
[52:14] Dispensed 0.000941 mL of Base (0.5 M KOH)
[52:20] Stepping pH = 5.37
[52:20] Dispensed 0.000071 mL of Base (0.5 M KOH)
[52:25] Stepping pH = 5.37
[52:25] Dispensed 0.000165 mL of Base (0.5 M KOH)
[52:30] Stepping pH = 5.41
[52:45] Stirrer speed set to 0
[52:55] Datapoint id 53 collected
[52:55] Charge balance equation is out by 37.1%
[52:55] Stirrer speed set to 55
[53:00] pH 5.40 -> 5.60
[53:00] Using cautious pH adjust
[53:00] Dispensed 0.000800 mL of Base (0.5 M KOH)
[53:05] Stepping pH = 5.62
[53:20] Stirrer speed set to 0
[53:31] Datapoint id 54 collected
[53:31] Charge balance equation is out by 50.0%
[53:31] Stirrer speed set to 55
[53:37] pH 5.62 -> 5.82
[53:37] Using cautious pH adjust
[53:37] Dispensed 0.000611 mL of Base (0.5 M KOH)
[53:42] Stepping pH = 5.83
[53:57] Stirrer speed set to 0
[54:07] Datapoint id 55 collected
[54:07] Charge balance equation is out by 50.0%
[54:07] Stirrer speed set to 55
[54:13] pH 5.84 -> 6.04
[54:13] Using cautious pH adjust
[54:13] Dispensed 0.000447 mL of Base (0.5 M KOH)
[54:18] Stepping pH = 6.07
[54:33] Stirrer speed set to 0
[54:44] Datapoint id 56 collected
[54:44] Charge balance equation is out by 50.0%

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[54:44] Stirrer speed set to 55
[54:49] pH 6.07 -> 6.27
[54:49] Using cautious pH adjust
[54:50] Dispensed 0.000306 mL of Base (0.5 M KOH)
[54:55] Stepping pH = 6.34
[55:10] Stirrer speed set to 0
[55:26] Datapoint id 57 collected
[55:26] Charge balance equation is out by 50.0%
[55:26] Stirrer speed set to 55
[55:31] pH 6.34 -> 6.54
[55:31] Using cautious pH adjust
[55:31] Dispensed 0.000188 mL of Base (0.5 M KOH)
[55:36] Stepping pH = 6.51
[55:36] Dispensed 0.000024 mL of Base (0.5 M KOH)
[55:41] Stepping pH = 6.54
[55:56] Stirrer speed set to 0
[56:11] Datapoint id 58 collected
[56:11] Charge balance equation is out by 43.1%
[56:11] Stirrer speed set to 55
[56:16] pH 6.54 -> 6.74
[56:16] Using cautious pH adjust
[56:16] Dispensed 0.000118 mL of Base (0.5 M KOH)
[56:22] Stepping pH = 6.69
[56:22] Dispensed 0.000024 mL of Base (0.5 M KOH)
[56:27] Stepping pH = 6.73
[56:42] Stirrer speed set to 0
[57:13] Datapoint id 59 collected
[57:13] Charge balance equation is out by 37.4%
[57:13] Stirrer speed set to 55
[57:18] pH 6.75 -> 6.95
[57:18] Using cautious pH adjust
[57:18] Dispensed 0.000094 mL of Base (0.5 M KOH)
[57:23] Stepping pH = 7.12
[57:38] Stirrer speed set to 0
[58:37] Datapoint id 60 collected
[58:37] Charge balance equation is out by 50.0%
[58:37] Stirrer speed set to 55
[58:42] pH 7.14 -> 7.34
[58:42] Using cautious pH adjust
[58:42] Dispensed 0.000047 mL of Base (0.5 M KOH)
[58:47] Stepping pH = 7.20
[58:48] Dispensed 0.000047 mL of Base (0.5 M KOH)
[58:53] Stepping pH = 7.55
[59:08] Stirrer speed set to 0
[1:00:08] Datapoint id 61 collected
[1:00:08] Charge balance equation is out by -6.7%
[1:00:08] Stirrer speed set to 55
[1:00:13] pH 7.60 -> 7.80
[1:00:13] Using charge balance adjust
[1:00:13] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:00:33] Stirrer speed set to 0
[1:01:27] Datapoint id 62 collected
[1:01:27] Charge balance equation is out by -85.7%
[1:01:27] Stirrer speed set to 55
[1:01:32] pH 7.69 -> 7.89
[1:01:32] Using cautious pH adjust
[1:01:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:37] Stepping pH = 7.73
[1:01:37] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:01:42] Stepping pH = 7.88
[1:01:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:01:47] Stepping pH = 8.02
[1:02:02] Stirrer speed set to 0
[1:03:01] Datapoint id 63 collected
[1:03:01] Charge balance equation is out by -137.8%
[1:03:01] Stirrer speed set to 55
[1:03:06] pH 8.09 -> 8.29
[1:03:06] Using cautious pH adjust
[1:03:06] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:11] Stepping pH = 8.15
[1:03:11] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:16] Stepping pH = 8.22
[1:03:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:03:21] Stepping pH = 8.32
[1:03:36] Stirrer speed set to 0
[1:04:21] Datapoint id 64 collected
[1:04:21] Charge balance equation is out by -239.8%
[1:04:21] Stirrer speed set to 55
[1:04:26] pH 8.40 -> 8.60
[1:04:26] Using cautious pH adjust
[1:04:27] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:32] Stepping pH = 8.43
[1:04:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:37] Stepping pH = 8.48
[1:04:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:42] Stepping pH = 8.55
[1:04:42] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:04:47] Stepping pH = 8.62
[1:05:02] Stirrer speed set to 0
[1:05:20] Datapoint id 65 collected
[1:05:20] Charge balance equation is out by -340.7%
[1:05:20] Stirrer speed set to 55
[1:05:25] pH 8.67 -> 8.87
[1:05:25] Using cautious pH adjust
[1:05:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:05:30] Stepping pH = 8.68
[1:05:30] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:05:36] Stepping pH = 8.75
[1:05:36] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:05:41] Stepping pH = 8.85
[1:05:41] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:05:46] Stepping pH = 8.89
[1:06:01] Stirrer speed set to 0
[1:06:22] Datapoint id 66 collected
[1:06:22] Charge balance equation is out by -302.4%
[1:06:22] Stirrer speed set to 55
[1:06:28] pH 8.90 -> 9.10
[1:06:28] Using cautious pH adjust
[1:06:28] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:06:33] Stepping pH = 8.91
[1:06:33] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:06:38] Stepping pH = 9.05
[1:06:38] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:06:43] Stepping pH = 9.08
[1:06:43] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:06:48] Stepping pH = 9.11
[1:07:03] Stirrer speed set to 0
[1:07:18] Datapoint id 67 collected

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:07:18] Charge balance equation is out by -180.0%
[1:07:18] Stirrer speed set to 55
[1:07:23] pH 9.12 -> 9.32
[1:07:23] Using cautious pH adjust
[1:07:23] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:07:28] Stepping pH = 9.16
[1:07:29] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:07:34] Stepping pH = 9.30
[1:07:34] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:07:39] Stepping pH = 9.31
[1:07:54] Stirrer speed set to 0
[1:08:04] Datapoint id 68 collected
[1:08:04] Charge balance equation is out by -73.1%
[1:08:04] Stirrer speed set to 55
[1:08:10] pH 9.32 -> 9.52
[1:08:10] Using cautious pH adjust
[1:08:10] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:08:15] Stepping pH = 9.36
[1:08:15] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:08:20] Stepping pH = 9.47
[1:08:20] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:08:25] Stepping pH = 9.50
[1:08:25] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:08:30] Stepping pH = 9.51
[1:08:45] Stirrer speed set to 0
[1:09:02] Datapoint id 69 collected
[1:09:02] Charge balance equation is out by -116.1%
[1:09:02] Stirrer speed set to 55
[1:09:07] pH 9.52 -> 9.72
[1:09:07] Using cautious pH adjust
[1:09:07] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:09:13] Stepping pH = 9.53
[1:09:13] Dispensed 0.000259 mL of Base (0.5 M KOH)
[1:09:18] Stepping pH = 9.76
[1:09:33] Stirrer speed set to 0
[1:09:49] Datapoint id 70 collected
[1:09:49] Charge balance equation is out by -89.8%
[1:09:49] Stirrer speed set to 55
[1:09:55] pH 9.76 -> 9.96
[1:09:55] Using cautious pH adjust
[1:09:55] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:10:00] Stepping pH = 9.82
[1:10:00] Dispensed 0.000212 mL of Base (0.5 M KOH)
[1:10:05] Stepping pH = 9.94
[1:10:05] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:10:10] Stepping pH = 9.95
[1:10:10] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:10:15] Stepping pH = 9.96
[1:10:30] Stirrer speed set to 0
[1:10:40] Datapoint id 71 collected
[1:10:40] Charge balance equation is out by -51.5%
[1:10:40] Stirrer speed set to 55
[1:10:45] pH 9.96 -> 10.05
[1:10:45] Using cautious pH adjust
[1:10:46] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:10:51] Stepping pH = 9.99
[1:10:51] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:10:56] Stepping pH = 10.02
[1:11:11] Stirrer speed set to 0

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:11:21] Datapoint id 72 collected
[1:11:21] Charge balance equation is out by -8.6%
[1:11:21] Titration 3 of 3
[1:11:21] Adding initial titrants
[1:11:21] Automatically add 0.30000 mL of Octanol
[1:11:28] Dispensed 0.300000 mL of Octanol
[1:11:28] Stirrer speed set to 10
[1:11:29] Stirrer speed set to 60
[1:11:29] Iterative adjust 10.02 -> 2.00
[1:11:29] pH 10.02 -> 2.00
[1:11:32] Dispensed 0.100000 mL of Acid (0.5 M HCl)
[1:11:37] pH 2.02 -> 2.00
[1:11:37] Dispensed 0.003881 mL of Acid (0.5 M HCl)
[1:12:27] Stirrer speed set to 0
[1:12:37] Datapoint id 73 collected
[1:12:37] Stirrer speed set to 60
[1:12:42] pH 1.98 -> 2.18
[1:12:42] Using cautious pH adjust
[1:12:43] Dispensed 0.015122 mL of Base (0.5 M KOH)
[1:12:48] Stepping pH = 2.07
[1:12:48] Dispensed 0.010160 mL of Base (0.5 M KOH)
[1:12:53] Stepping pH = 2.15
[1:12:54] Dispensed 0.002775 mL of Base (0.5 M KOH)
[1:12:59] Stepping pH = 2.18
[1:13:14] Stirrer speed set to 0
[1:13:24] Datapoint id 74 collected
[1:13:24] Charge balance equation is out by 7.3%
[1:13:24] Stirrer speed set to 60
[1:13:29] pH 2.19 -> 2.39
[1:13:29] Using charge balance adjust
[1:13:30] Dispensed 0.019450 mL of Base (0.5 M KOH)
[1:13:50] Stirrer speed set to 0
[1:14:00] Datapoint id 75 collected
[1:14:00] Charge balance equation is out by 6.0%
[1:14:00] Stirrer speed set to 60
[1:14:05] pH 2.40 -> 2.60
[1:14:05] Using charge balance adjust
[1:14:06] Dispensed 0.012700 mL of Base (0.5 M KOH)
[1:14:26] Stirrer speed set to 0
[1:14:36] Datapoint id 76 collected
[1:14:36] Charge balance equation is out by 11.5%
[1:14:36] Stirrer speed set to 60
[1:14:41] pH 2.63 -> 2.83
[1:14:41] Using charge balance adjust
[1:14:41] Dispensed 0.008443 mL of Base (0.5 M KOH)
[1:15:01] Stirrer speed set to 0
[1:15:11] Datapoint id 77 collected
[1:15:11] Charge balance equation is out by -0.8%
[1:15:11] Stirrer speed set to 60
[1:15:17] pH 2.83 -> 3.03
[1:15:17] Using charge balance adjust
[1:15:17] Dispensed 0.005974 mL of Base (0.5 M KOH)
[1:15:37] Stirrer speed set to 0
[1:15:47] Datapoint id 78 collected
[1:15:47] Charge balance equation is out by -2.6%
[1:15:47] Stirrer speed set to 60
[1:15:52] pH 3.03 -> 3.23
[1:15:52] Using charge balance adjust
[1:15:52] Dispensed 0.004280 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
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Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:16:12] Stirrer speed set to 0
[1:16:22] Datapoint id 79 collected
[1:16:22] Charge balance equation is out by 6.7%
[1:16:22] Stirrer speed set to 60
[1:16:28] pH 3.25 -> 3.45
[1:16:28] Using charge balance adjust
[1:16:28] Dispensed 0.003010 mL of Base (0.5 M KOH)
[1:16:48] Stirrer speed set to 0
[1:16:59] Datapoint id 80 collected
[1:16:59] Charge balance equation is out by -9.4%
[1:16:59] Stirrer speed set to 60
[1:17:04] pH 3.43 -> 3.63
[1:17:04] Using charge balance adjust
[1:17:04] Dispensed 0.002305 mL of Base (0.5 M KOH)
[1:17:24] Stirrer speed set to 0
[1:17:39] Datapoint id 81 collected
[1:17:39] Charge balance equation is out by -27.6%
[1:17:39] Stirrer speed set to 60
[1:17:44] pH 3.57 -> 3.77
[1:17:44] Using cautious pH adjust
[1:17:44] Dispensed 0.000988 mL of Base (0.5 M KOH)
[1:17:49] Stepping pH = 3.65
[1:17:49] Dispensed 0.000917 mL of Base (0.5 M KOH)
[1:17:55] Stepping pH = 3.73
[1:17:55] Dispensed 0.000423 mL of Base (0.5 M KOH)
[1:18:00] Stepping pH = 3.76
[1:18:00] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:18:05] Stepping pH = 3.77
[1:18:20] Stirrer speed set to 0
[1:18:30] Datapoint id 82 collected
[1:18:30] Charge balance equation is out by -24.4%
[1:18:30] Stirrer speed set to 60
[1:18:35] pH 3.76 -> 3.96
[1:18:35] Using cautious pH adjust
[1:18:35] Dispensed 0.000870 mL of Base (0.5 M KOH)
[1:18:40] Stepping pH = 3.85
[1:18:40] Dispensed 0.000706 mL of Base (0.5 M KOH)
[1:18:46] Stepping pH = 3.91
[1:18:46] Dispensed 0.000400 mL of Base (0.5 M KOH)
[1:18:51] Stepping pH = 3.94
[1:18:51] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:18:56] Stepping pH = 3.95
[1:19:11] Stirrer speed set to 0
[1:19:21] Datapoint id 83 collected
[1:19:21] Charge balance equation is out by -24.7%
[1:19:21] Stirrer speed set to 60
[1:19:26] pH 3.94 -> 4.14
[1:19:26] Using cautious pH adjust
[1:19:26] Dispensed 0.000847 mL of Base (0.5 M KOH)
[1:19:31] Stepping pH = 4.01
[1:19:31] Dispensed 0.000917 mL of Base (0.5 M KOH)
[1:19:37] Stepping pH = 4.09
[1:19:37] Dispensed 0.000447 mL of Base (0.5 M KOH)
[1:19:42] Stepping pH = 4.12
[1:19:42] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:19:47] Stepping pH = 4.13
[1:20:02] Stirrer speed set to 0
[1:20:12] Datapoint id 84 collected
[1:20:12] Charge balance equation is out by -41.6%

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:20:12] Stirrer speed set to 60
[1:20:17] pH 4.11 -> 4.31
[1:20:17] Using cautious pH adjust
[1:20:17] Dispensed 0.000894 mL of Base (0.5 M KOH)
[1:20:22] Stepping pH = 4.19
[1:20:22] Dispensed 0.000823 mL of Base (0.5 M KOH)
[1:20:28] Stepping pH = 4.27
[1:20:28] Dispensed 0.000329 mL of Base (0.5 M KOH)
[1:20:33] Stepping pH = 4.30
[1:20:33] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:20:38] Stepping pH = 4.30
[1:20:53] Stirrer speed set to 0
[1:21:03] Datapoint id 85 collected
[1:21:03] Charge balance equation is out by -23.0%
[1:21:03] Stirrer speed set to 60
[1:21:08] pH 4.29 -> 4.49
[1:21:08] Using cautious pH adjust
[1:21:08] Dispensed 0.000964 mL of Base (0.5 M KOH)
[1:21:13] Stepping pH = 4.39
[1:21:14] Dispensed 0.000706 mL of Base (0.5 M KOH)
[1:21:19] Stepping pH = 4.47
[1:21:19] Dispensed 0.000188 mL of Base (0.5 M KOH)
[1:21:24] Stepping pH = 4.49
[1:21:39] Stirrer speed set to 0
[1:21:49] Datapoint id 86 collected
[1:21:49] Charge balance equation is out by 3.5%
[1:21:49] Stirrer speed set to 60
[1:21:55] pH 4.47 -> 4.67
[1:21:55] Using charge balance adjust
[1:21:55] Dispensed 0.002046 mL of Base (0.5 M KOH)
[1:22:15] Stirrer speed set to 0
[1:22:25] Datapoint id 87 collected
[1:22:25] Charge balance equation is out by 40.8%
[1:22:25] Stirrer speed set to 60
[1:22:31] pH 4.75 -> 4.95
[1:22:31] Using cautious pH adjust
[1:22:31] Dispensed 0.001035 mL of Base (0.5 M KOH)
[1:22:36] Stepping pH = 4.93
[1:22:36] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:22:41] Stepping pH = 4.94
[1:22:56] Stirrer speed set to 0
[1:23:07] Datapoint id 88 collected
[1:23:07] Charge balance equation is out by 45.1%
[1:23:07] Stirrer speed set to 60
[1:23:12] pH 4.93 -> 5.13
[1:23:12] Using cautious pH adjust
[1:23:12] Dispensed 0.000941 mL of Base (0.5 M KOH)
[1:23:17] Stepping pH = 5.13
[1:23:32] Stirrer speed set to 0
[1:23:42] Datapoint id 89 collected
[1:23:42] Charge balance equation is out by 50.0%
[1:23:42] Stirrer speed set to 60
[1:23:47] pH 5.11 -> 5.31
[1:23:47] Using cautious pH adjust
[1:23:47] Dispensed 0.000800 mL of Base (0.5 M KOH)
[1:23:52] Stepping pH = 5.34
[1:24:07] Stirrer speed set to 0
[1:24:24] Datapoint id 90 collected
[1:24:24] Charge balance equation is out by 50.0%

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
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Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:24:24] Stirrer speed set to 60
[1:24:30] pH 5.32 -> 5.52
[1:24:30] Using cautious pH adjust
[1:24:30] Dispensed 0.000611 mL of Base (0.5 M KOH)
[1:24:35] Stepping pH = 5.57
[1:24:50] Stirrer speed set to 0
[1:25:01] Datapoint id 91 collected
[1:25:01] Charge balance equation is out by 50.0%
[1:25:01] Stirrer speed set to 60
[1:25:06] pH 5.56 -> 5.76
[1:25:06] Using cautious pH adjust
[1:25:06] Dispensed 0.000423 mL of Base (0.5 M KOH)
[1:25:11] Stepping pH = 5.85
[1:25:26] Stirrer speed set to 0
[1:25:39] Datapoint id 92 collected
[1:25:39] Charge balance equation is out by 50.0%
[1:25:39] Stirrer speed set to 60
[1:25:44] pH 5.85 -> 6.05
[1:25:44] Using cautious pH adjust
[1:25:44] Dispensed 0.000259 mL of Base (0.5 M KOH)
[1:25:49] Stepping pH = 6.16
[1:26:04] Stirrer speed set to 0
[1:26:35] Datapoint id 93 collected
[1:26:35] Charge balance equation is out by 50.0%
[1:26:35] Stirrer speed set to 60
[1:26:40] pH 6.11 -> 6.31
[1:26:40] Using cautious pH adjust
[1:26:40] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:26:46] Stepping pH = 6.42
[1:27:01] Stirrer speed set to 0
[1:27:43] Datapoint id 94 collected
[1:27:43] Charge balance equation is out by 50.0%
[1:27:43] Stirrer speed set to 60
[1:27:48] pH 6.39 -> 6.59
[1:27:48] Using cautious pH adjust
[1:27:48] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:27:53] Stepping pH = 6.50
[1:27:53] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:27:58] Stepping pH = 6.74
[1:28:13] Stirrer speed set to 0
[1:29:09] Datapoint id 95 collected
[1:29:09] Charge balance equation is out by 21.9%
[1:29:09] Stirrer speed set to 60
[1:29:14] pH 6.69 -> 6.89
[1:29:14] Using cautious pH adjust
[1:29:14] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:29:20] Stepping pH = 6.88
[1:29:20] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:29:25] Stepping pH = 6.99
[1:29:40] Stirrer speed set to 0
[1:30:40] Datapoint id 96 collected
[1:30:40] Charge balance equation is out by 34.4%
[1:30:40] Stirrer speed set to 60
[1:30:45] pH 7.00 -> 7.20
[1:30:45] Using cautious pH adjust
[1:30:45] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:30:50] Stepping pH = 7.14
[1:30:50] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:30:55] Stepping pH = 7.32

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:31:11] Stirrer speed set to 0
[1:32:11] Datapoint id 97 collected
[1:32:11] Charge balance equation is out by 22.4%
[1:32:11] Stirrer speed set to 60
[1:32:16] pH 7.20 -> 7.40
[1:32:16] Using cautious pH adjust
[1:32:16] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:32:21] Stepping pH = 7.16
[1:32:21] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:32:26] Stepping pH = 8.36
[1:32:41] Stirrer speed set to 0
[1:33:41] Datapoint id 98 collected
[1:33:41] Charge balance equation is out by -248.0%
[1:33:41] Stirrer speed set to 60
[1:33:46] pH 8.32 -> 8.52
[1:33:46] Using cautious pH adjust
[1:33:46] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:33:51] Stepping pH = 8.32
[1:33:51] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:33:56] Stepping pH = 8.34
[1:33:57] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:34:02] Stepping pH = 8.63
[1:34:17] Stirrer speed set to 0
[1:34:34] Datapoint id 99 collected
[1:34:34] Charge balance equation is out by -554.6%
[1:34:34] Stirrer speed set to 60
[1:34:39] pH 8.67 -> 8.87
[1:34:39] Using cautious pH adjust
[1:34:39] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:34:45] Stepping pH = 8.67
[1:34:45] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:34:50] Stepping pH = 8.72
[1:34:50] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:34:55] Stepping pH = 8.88
[1:35:10] Stirrer speed set to 0
[1:35:31] Datapoint id 100 collected
[1:35:31] Charge balance equation is out by -321.4%
[1:35:31] Stirrer speed set to 60
[1:35:37] pH 8.92 -> 9.12
[1:35:37] Using cautious pH adjust
[1:35:37] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:35:42] Stepping pH = 8.92
[1:35:42] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:35:47] Stepping pH = 9.04
[1:35:47] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:35:52] Stepping pH = 9.08
[1:35:52] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:35:57] Stepping pH = 9.13
[1:36:12] Stirrer speed set to 0
[1:36:24] Datapoint id 101 collected
[1:36:24] Charge balance equation is out by -240.5%
[1:36:24] Stirrer speed set to 60
[1:36:29] pH 9.12 -> 9.32
[1:36:29] Using cautious pH adjust
[1:36:29] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:36:34] Stepping pH = 9.14
[1:36:34] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:36:39] Stepping pH = 9.30
[1:36:39] Dispensed 0.000024 mL of Base (0.5 M KOH)

Sample name: **M15_octanol**
Assay name: **pH-metric high logP**
Assay ID: **18B-28002**
Filename: **C:\Sirius_T3\Mehtap\20180227_exp27_logP_T3-2\18B-28002_M15_octanol_pH-metric high logP.t3r**

Experiment start time: **2/28/2018 1:10:47 AM**
Analyst: **Pion**
Instrument ID: **T312060**

Experiment Log (continued)

[1:36:44] Stepping pH = 9.31
[1:37:00] Stirrer speed set to 0
[1:37:12] Datapoint id 102 collected
[1:37:12] Charge balance equation is out by -99.8%
[1:37:12] Stirrer speed set to 60
[1:37:17] pH 9.31 -> 9.51
[1:37:17] Using cautious pH adjust
[1:37:17] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:37:22] Stepping pH = 9.35
[1:37:22] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:37:27] Stepping pH = 9.48
[1:37:27] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:37:32] Stepping pH = 9.50
[1:37:32] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:37:37] Stepping pH = 9.52
[1:37:52] Stirrer speed set to 0
[1:38:03] Datapoint id 103 collected
[1:38:03] Charge balance equation is out by -92.7%
[1:38:03] Stirrer speed set to 60
[1:38:09] pH 9.52 -> 9.72
[1:38:09] Using cautious pH adjust
[1:38:09] Dispensed 0.000094 mL of Base (0.5 M KOH)
[1:38:14] Stepping pH = 9.59
[1:38:14] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:38:19] Stepping pH = 9.68
[1:38:19] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:38:24] Stepping pH = 9.70
[1:38:24] Dispensed 0.000047 mL of Base (0.5 M KOH)
[1:38:29] Stepping pH = 9.72
[1:38:44] Stirrer speed set to 0
[1:38:54] Datapoint id 104 collected
[1:38:54] Charge balance equation is out by -63.5%
[1:38:54] Stirrer speed set to 60
[1:38:59] pH 9.73 -> 9.93
[1:38:59] Using cautious pH adjust
[1:38:59] Dispensed 0.000141 mL of Base (0.5 M KOH)
[1:39:05] Stepping pH = 9.81
[1:39:05] Dispensed 0.000165 mL of Base (0.5 M KOH)
[1:39:10] Stepping pH = 9.90
[1:39:10] Dispensed 0.000071 mL of Base (0.5 M KOH)
[1:39:15] Stepping pH = 9.92
[1:39:15] Dispensed 0.000024 mL of Base (0.5 M KOH)
[1:39:20] Stepping pH = 9.93
[1:39:35] Stirrer speed set to 0
[1:39:46] Datapoint id 105 collected
[1:39:46] Charge balance equation is out by -32.3%
[1:39:46] Stirrer speed set to 60
[1:39:51] pH 9.93 -> 10.05
[1:39:51] Using cautious pH adjust
[1:39:51] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:39:56] Stepping pH = 9.98
[1:39:56] Dispensed 0.000118 mL of Base (0.5 M KOH)
[1:40:01] Stepping pH = 10.03
[1:40:16] Stirrer speed set to 0
[1:40:27] Datapoint id 106 collected
[1:40:27] Charge balance equation is out by 0.6%
[1:40:27] Argon flow rate set to 0
[1:40:31] Titrator arm moved over Titration position